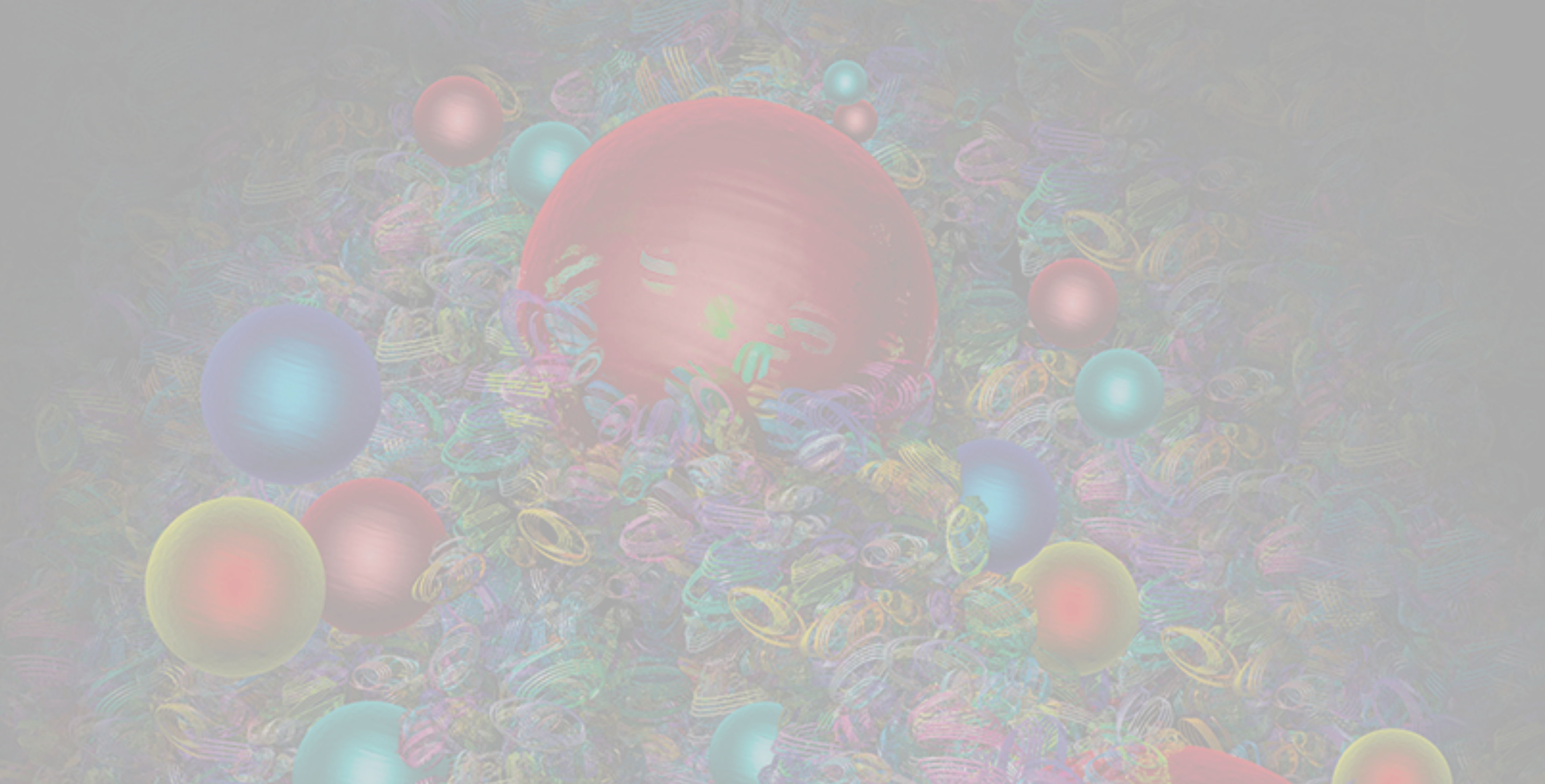
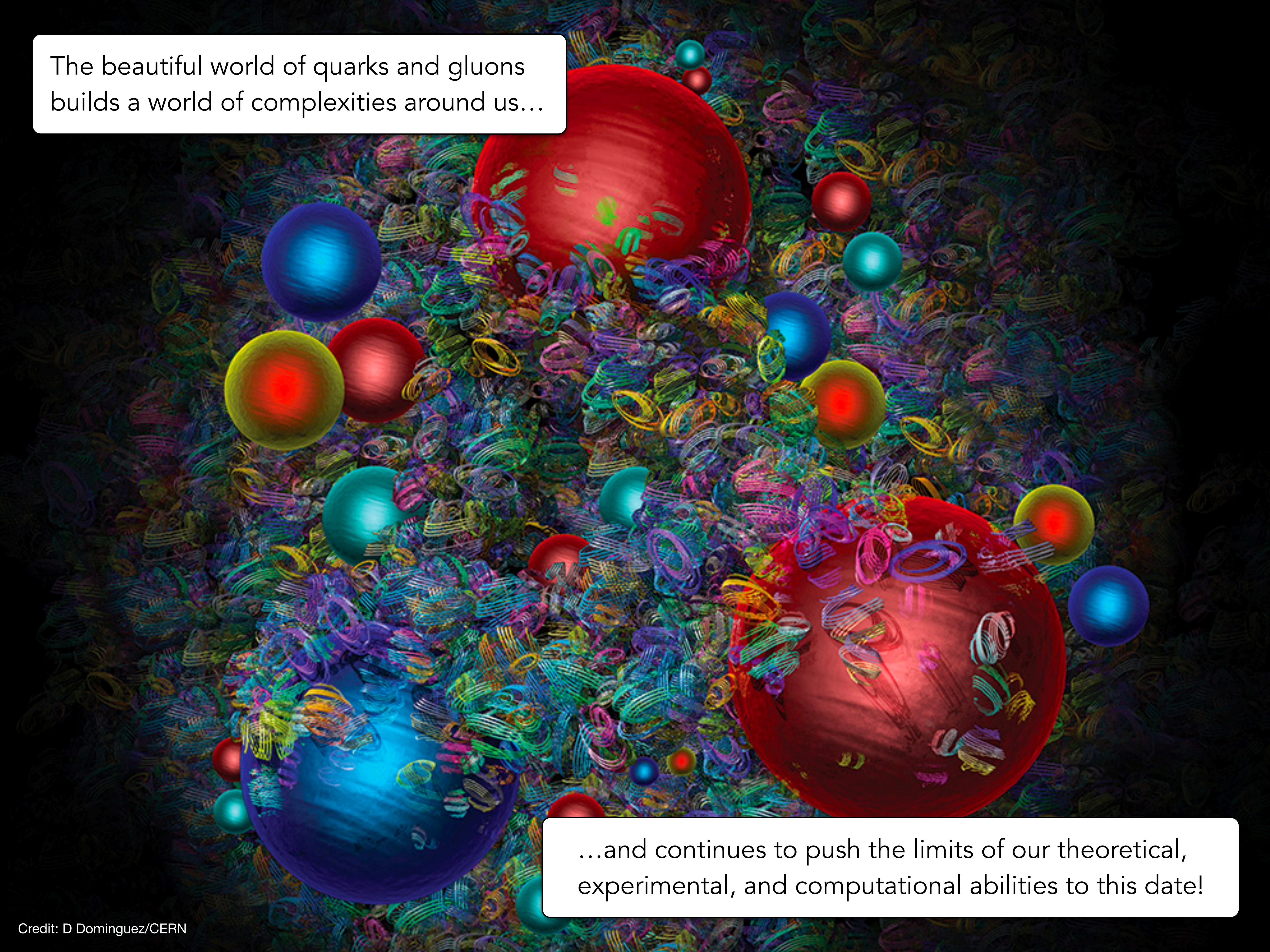


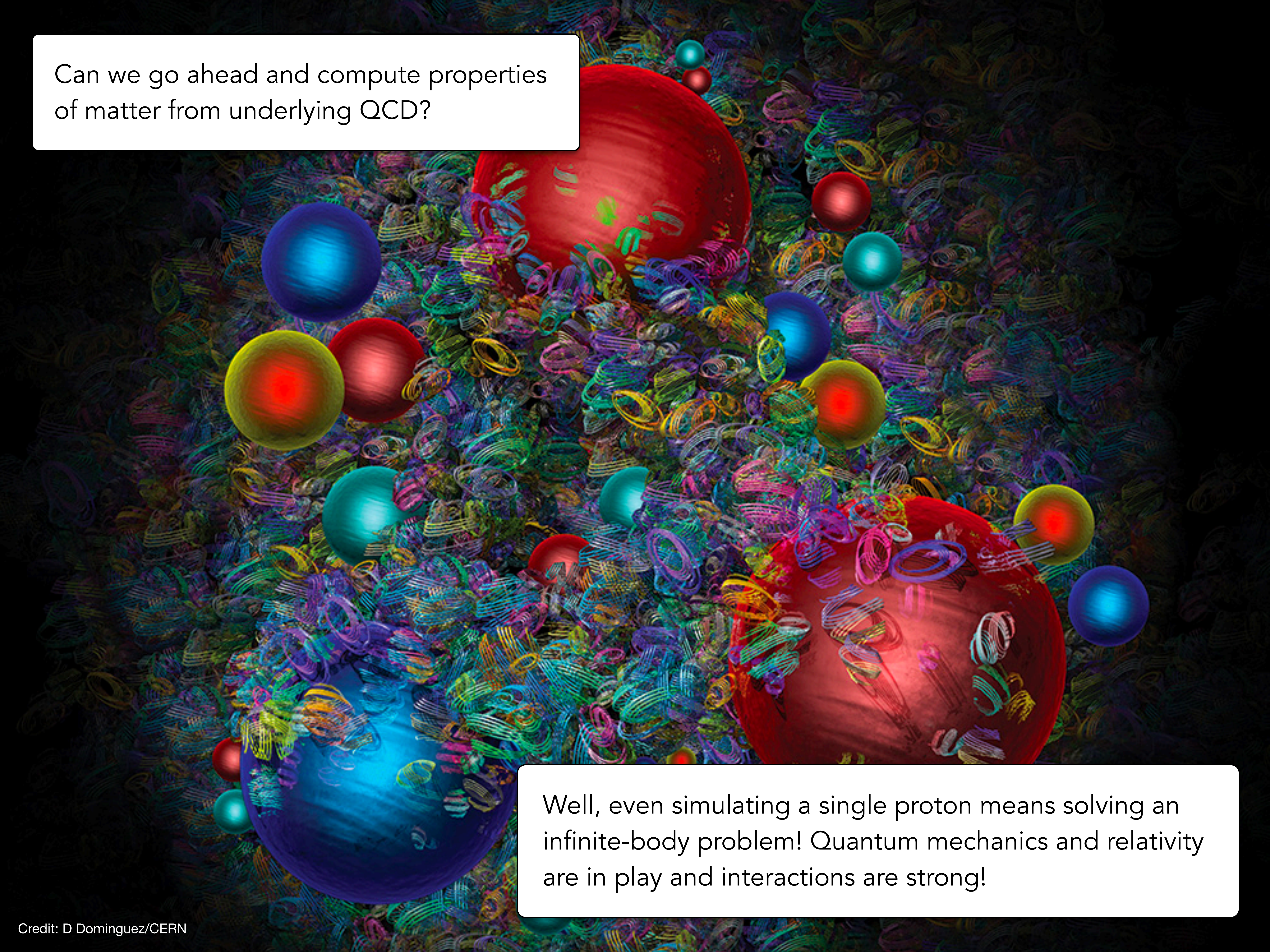
[Remote] Talk @ the XVth Quark Confinement and
the Hadron Spectrum Conference
University of Stavanger, Norway
Aug 1-6, 2022

Quantum simulations for QCD: Where we are now and what is in reach

Zohreh Davoudi
University of Maryland, College Park


The beautiful world of quarks and gluons builds a world of complexities around us…
…and continues to push the limits of our theoretical, experimental, and computational abilities to this date!
Credit: D Dominguez/CERN

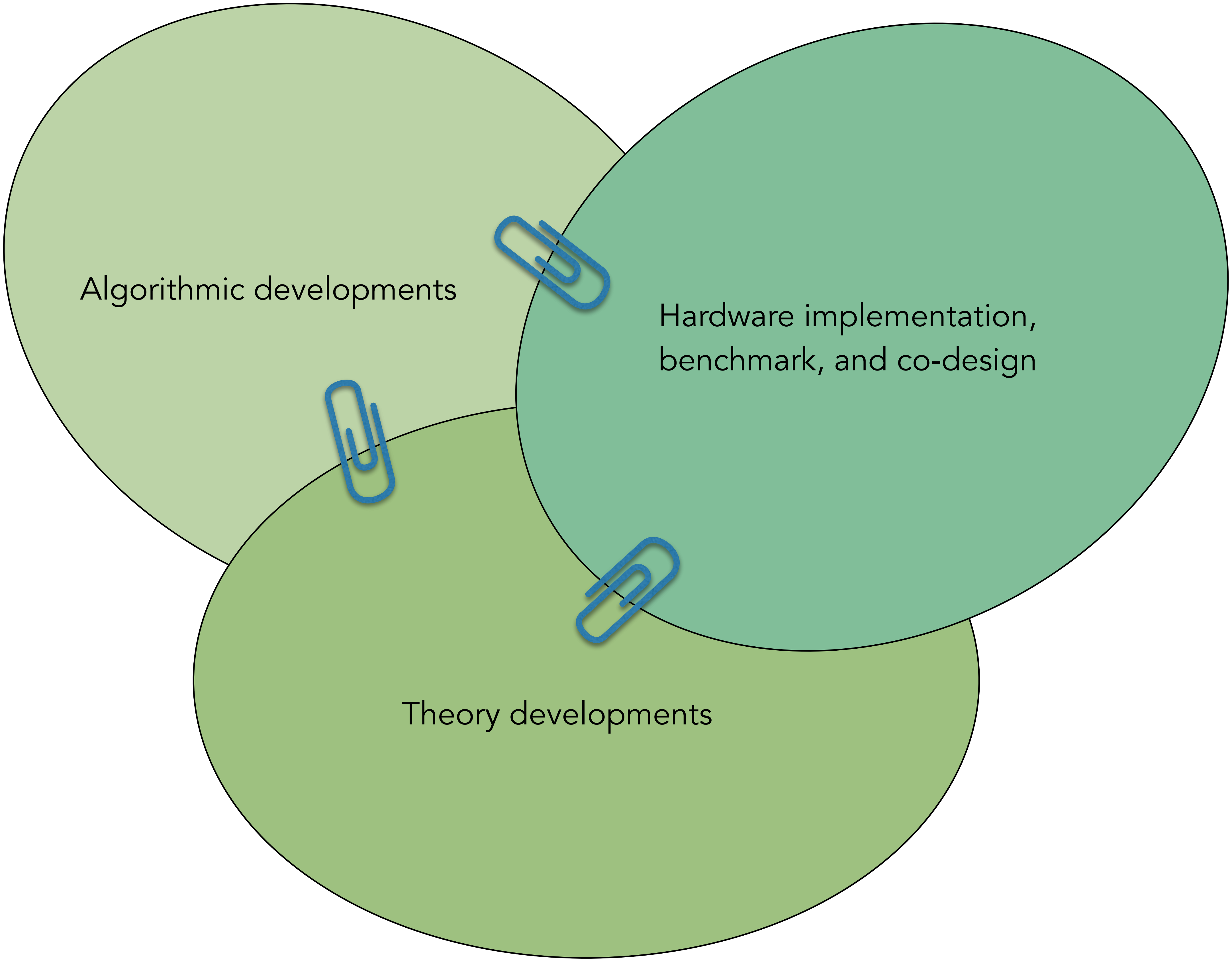
Can we go ahead and compute properties of matter from underlying QCD?



Well, even simulating a single proton means solving an infinite-body problem! Quantum mechanics and relativity are in play and interactions are strong!

Credit: D Dominguez/CERN

LATTICE QCD: A MULTI-PRONG PROGRAM THAT SIMULATES QCD NON-PERTURBATIVELY



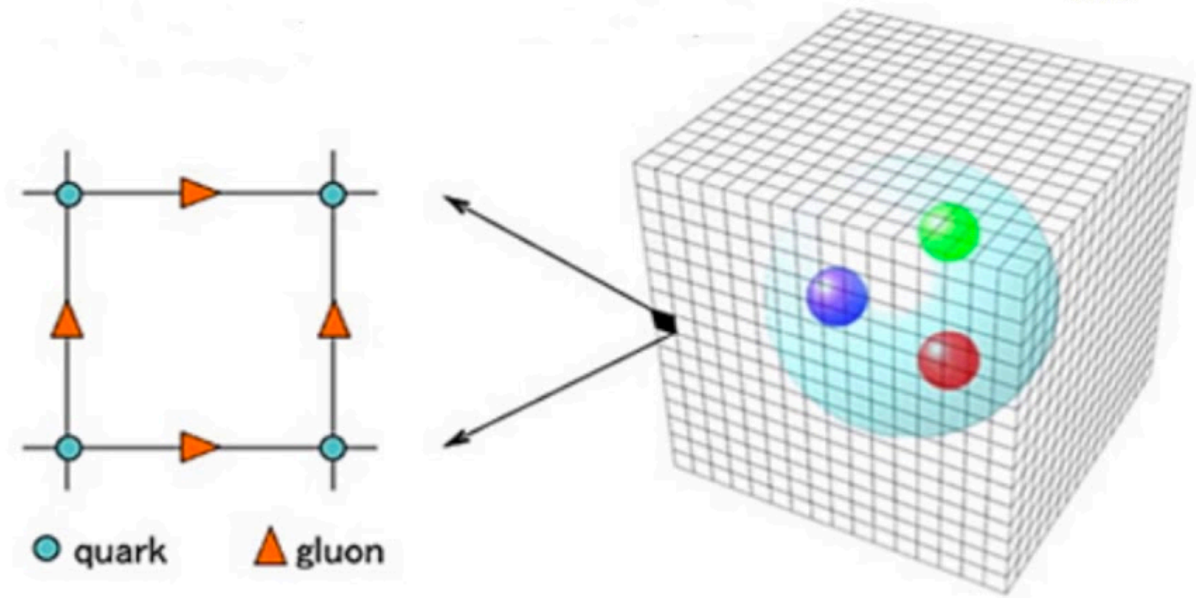
Theory developments

How to define QCD/QED on a finite grid?

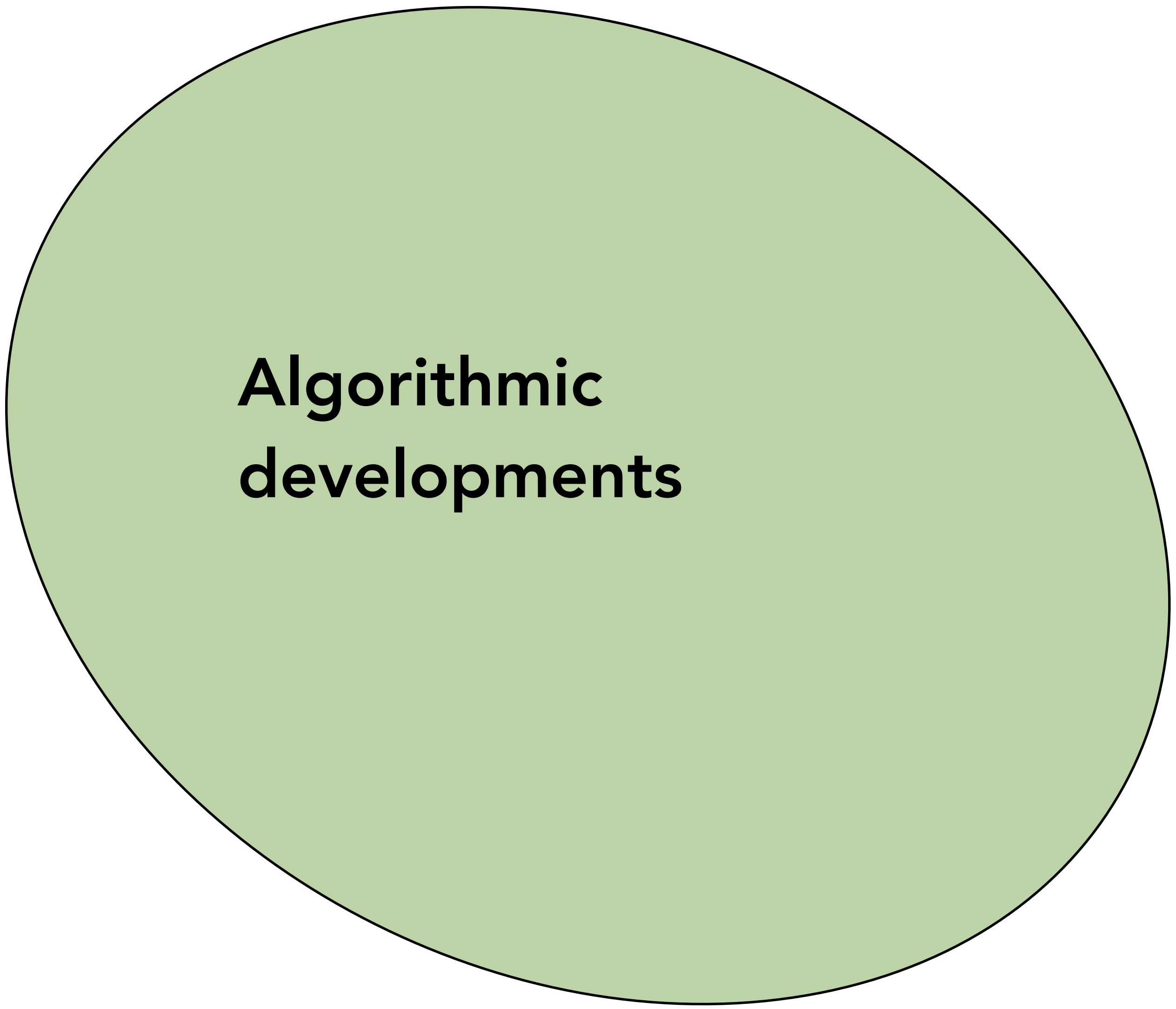
How to preserve/recover symmetries,
e.g., gauge symmetry, chiral symmetry,
rotational symmetry.

How to take infinite-volume and continuum limits? How to quantify systematics?

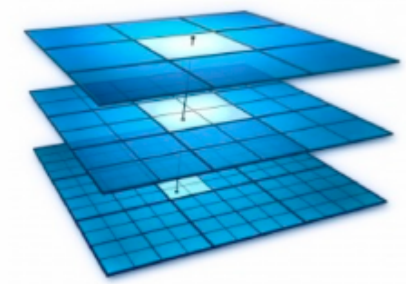
How to obtain scattering amplitudes
and decay rates?



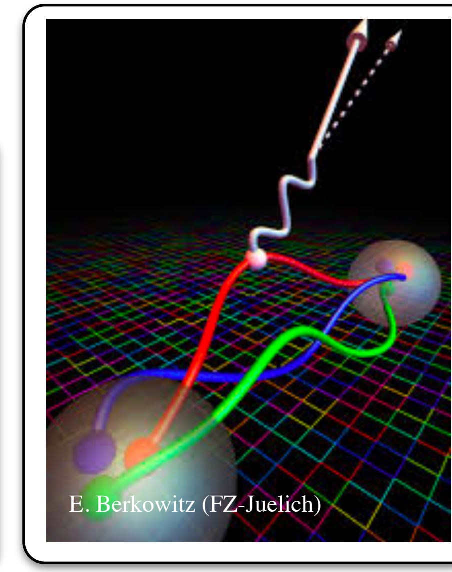
Theory developments

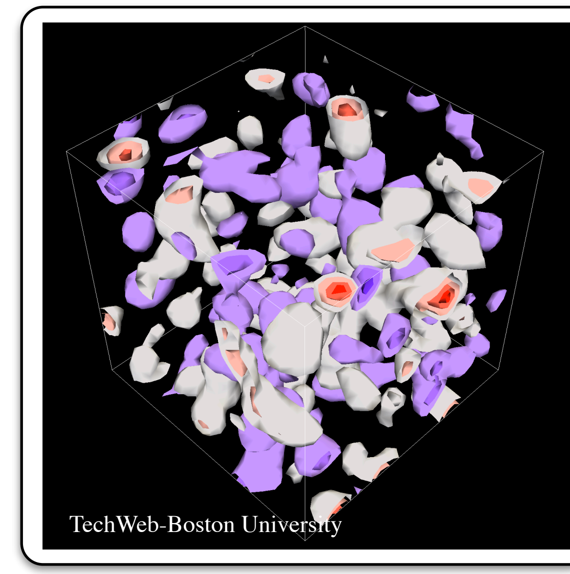

Algorithmic
developments

Algorithmic developments



e.g. How to solve **optimally** ? A.x=b



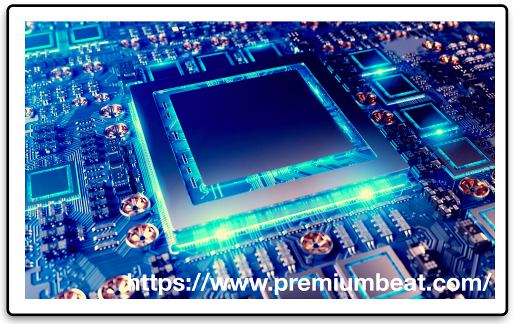


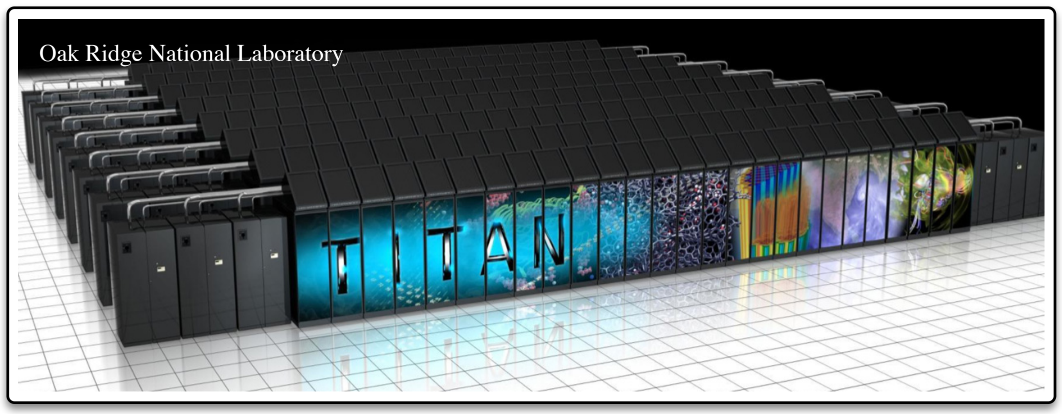
How to importance sample vacuum gauge configurations?

How to evaluate quark propagators (invert large matrices)?

How to contract quarks and form correlation functions efficiently?

Implementation, benchmark, and co-design





Implementation, benchmark, and co-design

Which tasks can be parallelized and which tasks are done in series?

What are the memory requirements and what kind of node connectivity is required?

Can we take advantage of GPUs? Which parts of the computations are more suitable for given architecture?

QCD ON A CHIP!

534 Nuclear Instruments and Methods in Physics Research 222 (1984) 534–539
North-Holland, Amsterdam

HARDWARE MATRIX MULTIPLIER / ACCUMULATOR FOR LATTICE GAUGE THEORY CALCULATIONS *

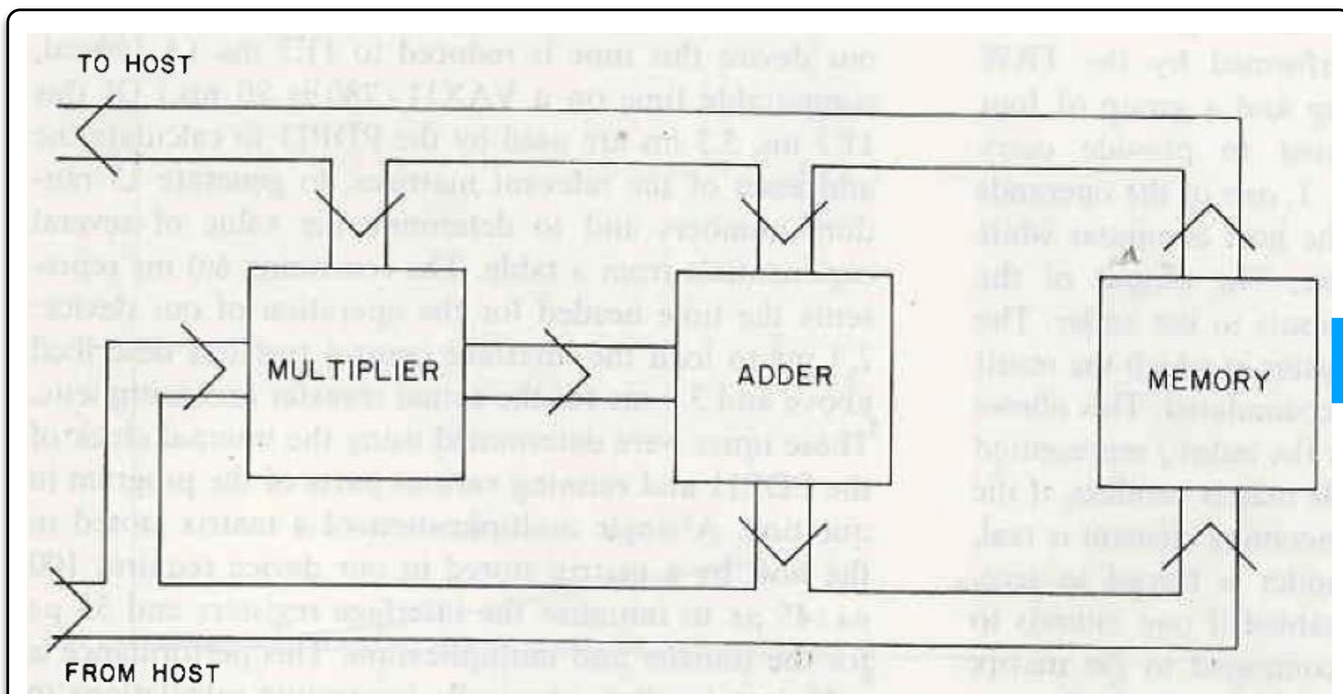
Norman H. CHRIST and Anthony E. TERRANO

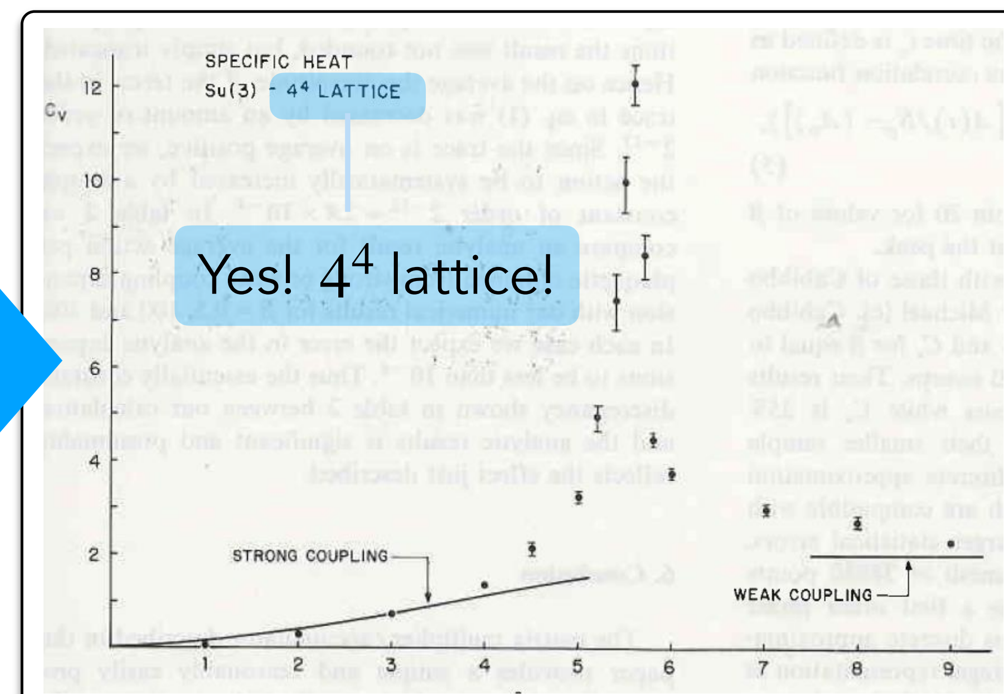
Columbia University, New York, NY 10027, USA

Received 30 September 1983

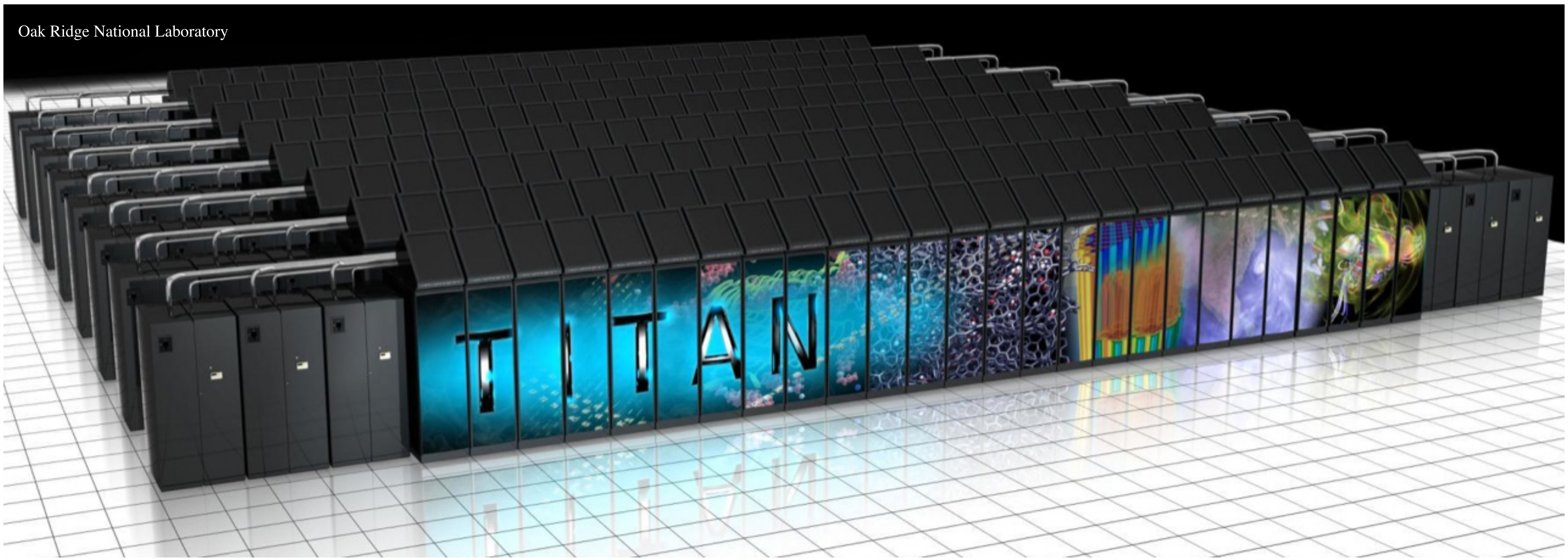
~40 years ago!

10^{10} times or more slower than current supercomputers!
Only few Kbytes of memory!





PUTTING ALL THESE HEROIC THEORY, ALGORITHM, AND CO-DESIGN EFFORTS TO WORK AND HAVING ACCESS TO HUNDREDS OF MILLION CPU HOURS ON THE LARGEST SUPERCOMPUTERS IN THE WORLD…

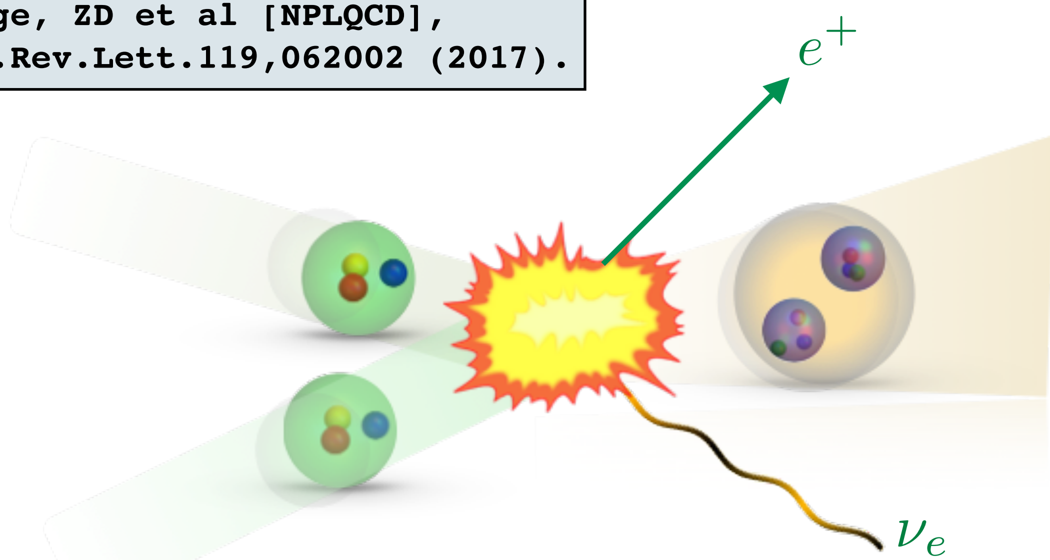


Titan supercomputer, Oak Ridge National Laboratory, USA

HAS LED TO TENS OF SUCCESS EXAMPLES BUT LET ME TELL YOU ABOUT ONE...

pp fusion cross section

Savage, ZD et al [NPLQCD], Phys.Rev.Lett.119,062002 (2017).



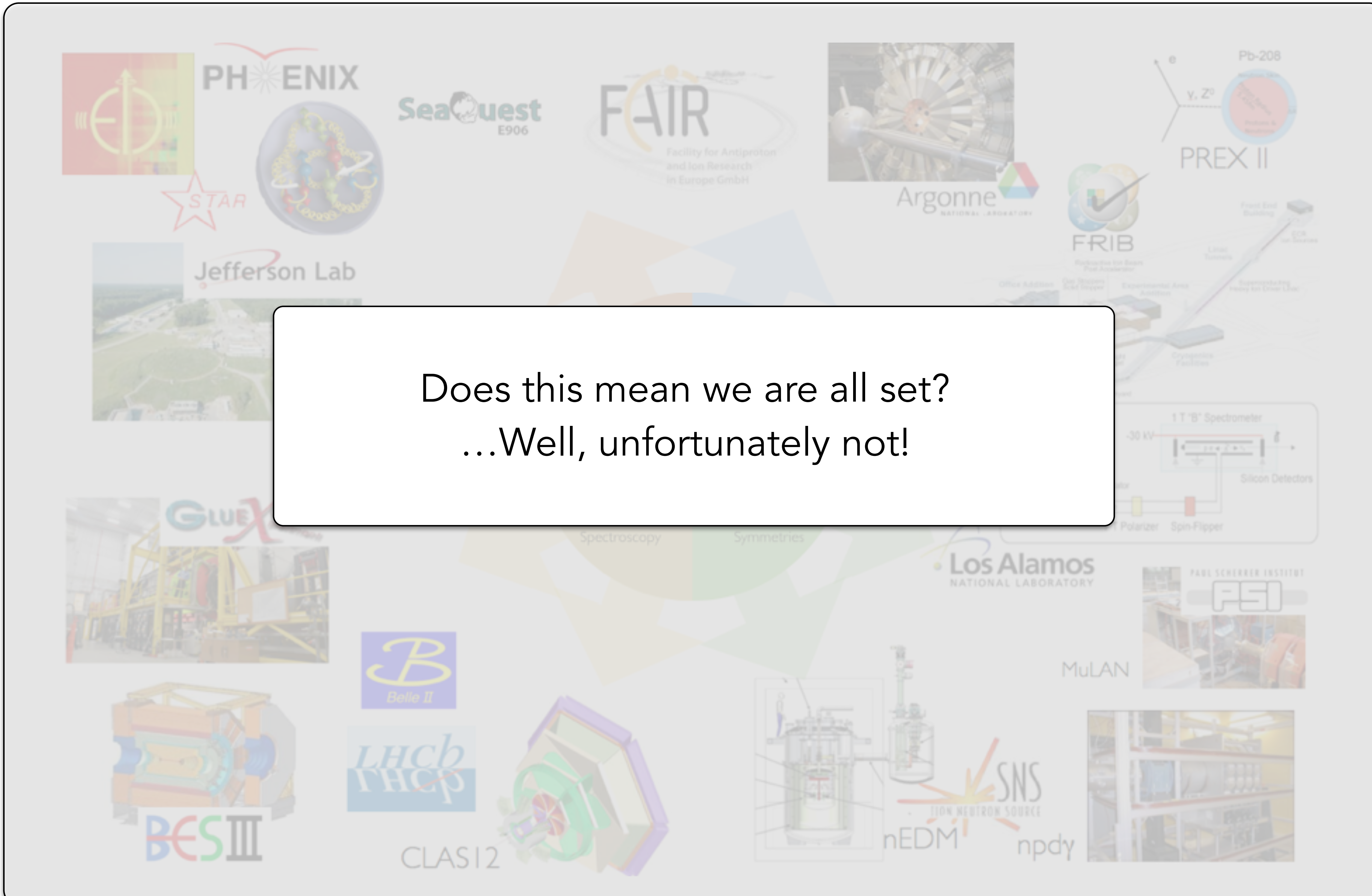
$$L_{1,A} = 3.9(0.1)(1.0)(0.3)(0.9)\ \mathrm{fm}^3 \ \ @\ \mu = m_\pi^{\mathrm{phys.}} = 140\ \mathrm{MeV}$$

ZD, Detmold, Orginos, Parreño, Savage, Shanahan, Wagman, *Phys.Rept.*900,1-74 (2021).

LATTICE QCD IS SUPPORTING A MULTI-BILLION DOLLAR EXPERIMENTAL PROGRAM!

Slide content courtesy of Martin Savage.

LATTICE QCD IS SUPPORTING A MULTI-BILLION DOLLAR EXPERIMENTAL PROGRAM!

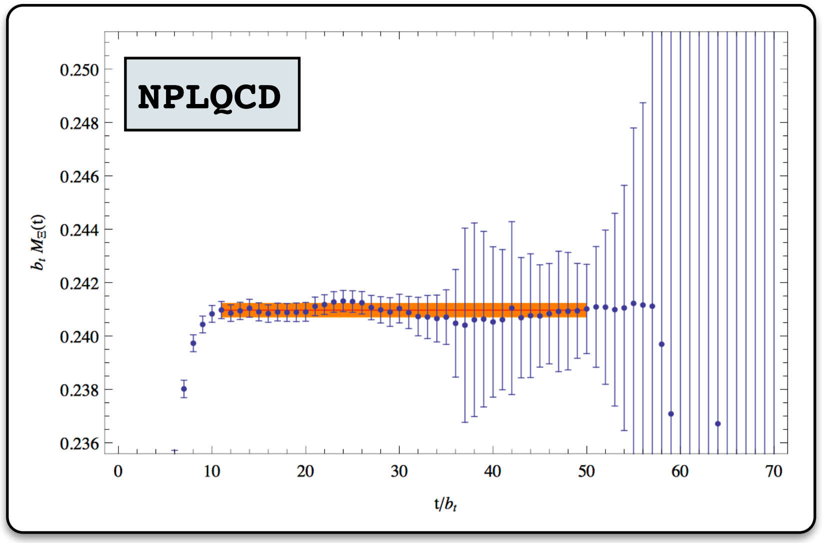


Does this mean we are all set?
…Well, unfortunately not!

Slide content courtesy of Martin Savage.

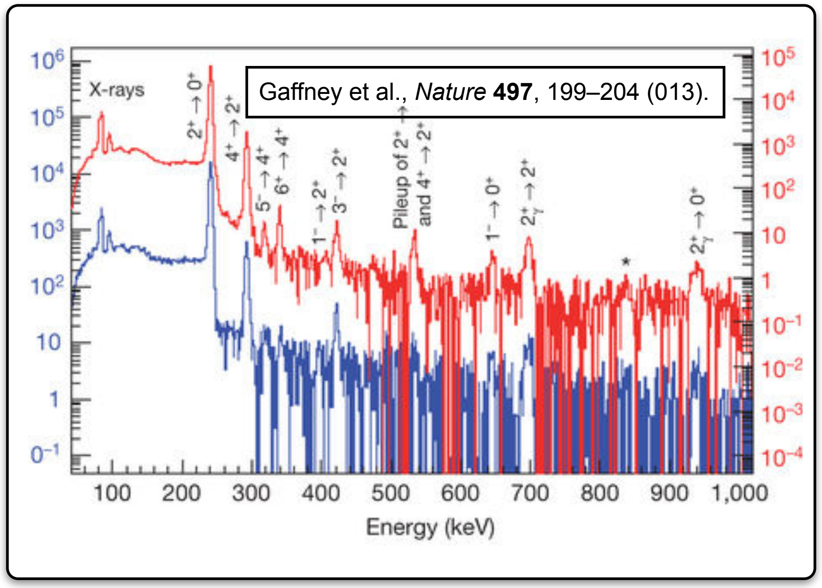
THREE FEATURES MAKE LATTICE QCD CALCULATIONS OF NUCLEI HARD:

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



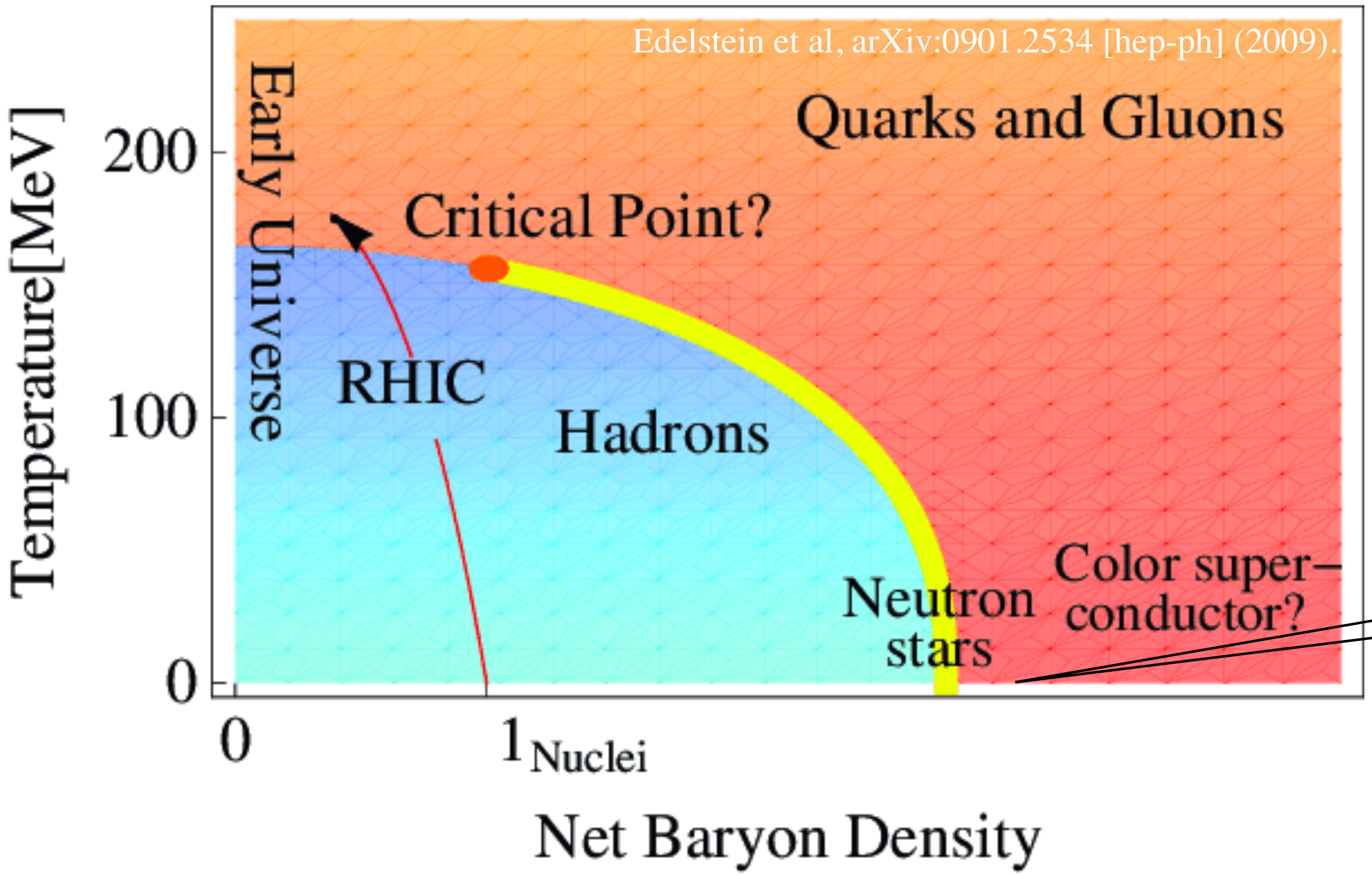
ii) There is a severe signal-to-noise degradation.

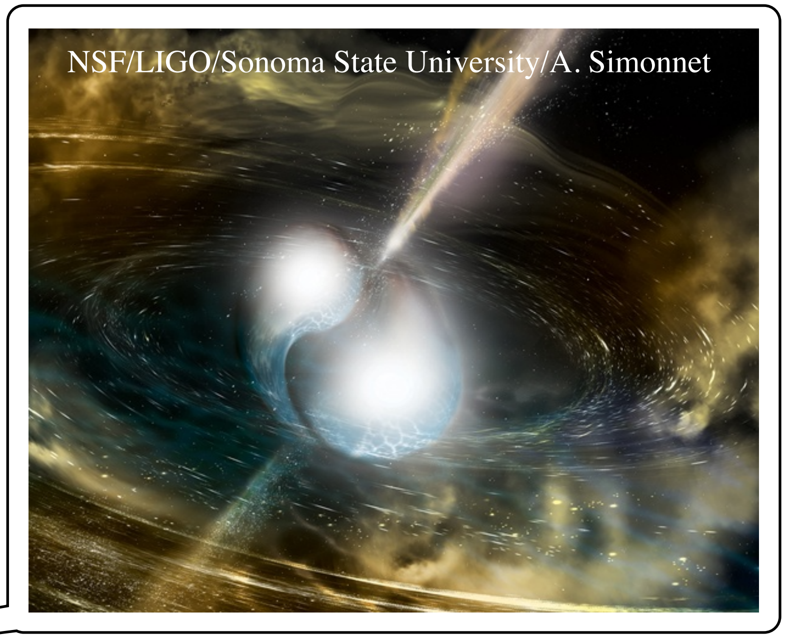
iii) Excitation energies of nuclei are much smaller than the QCD scale.



ADDITIONALLY THE SIGN PROBLEM FORBIDS:

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





Path integral formulation:

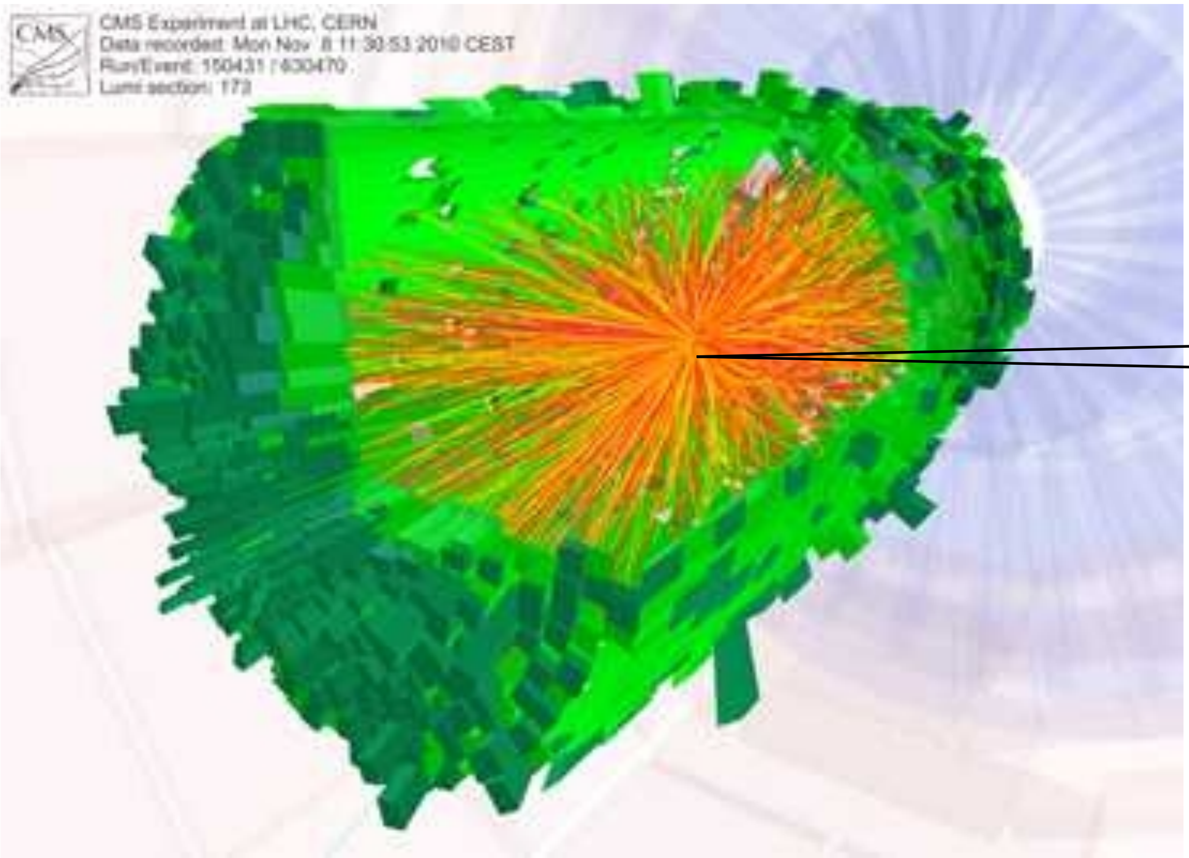
$$e^{-S[U,q,\bar{q}]}$$

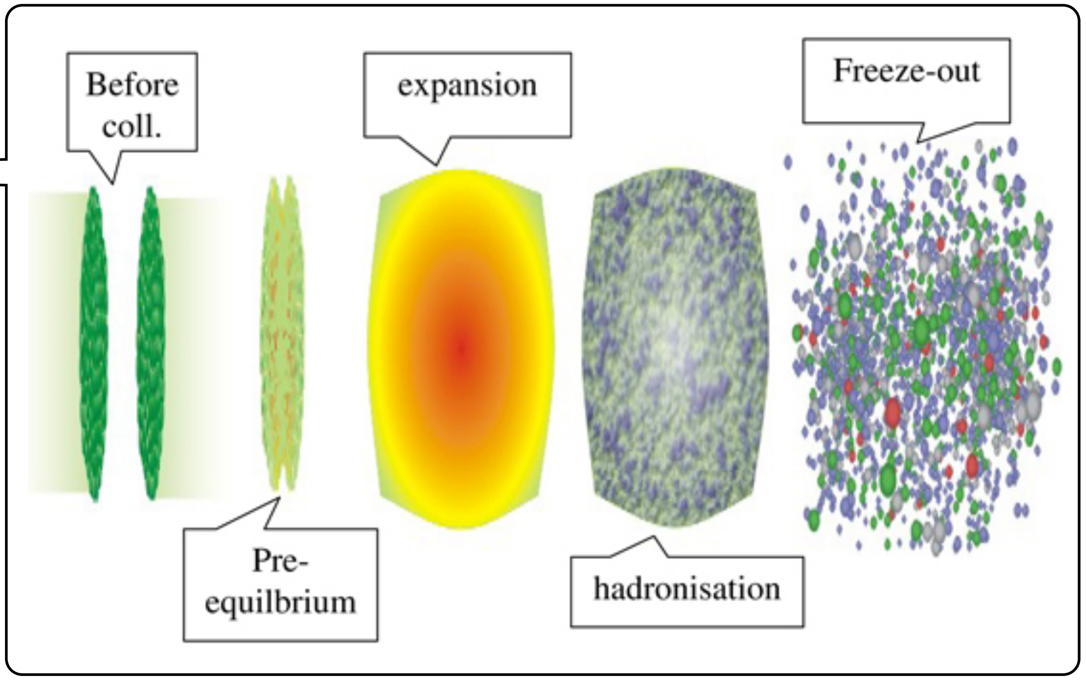
with a complex action:

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

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.

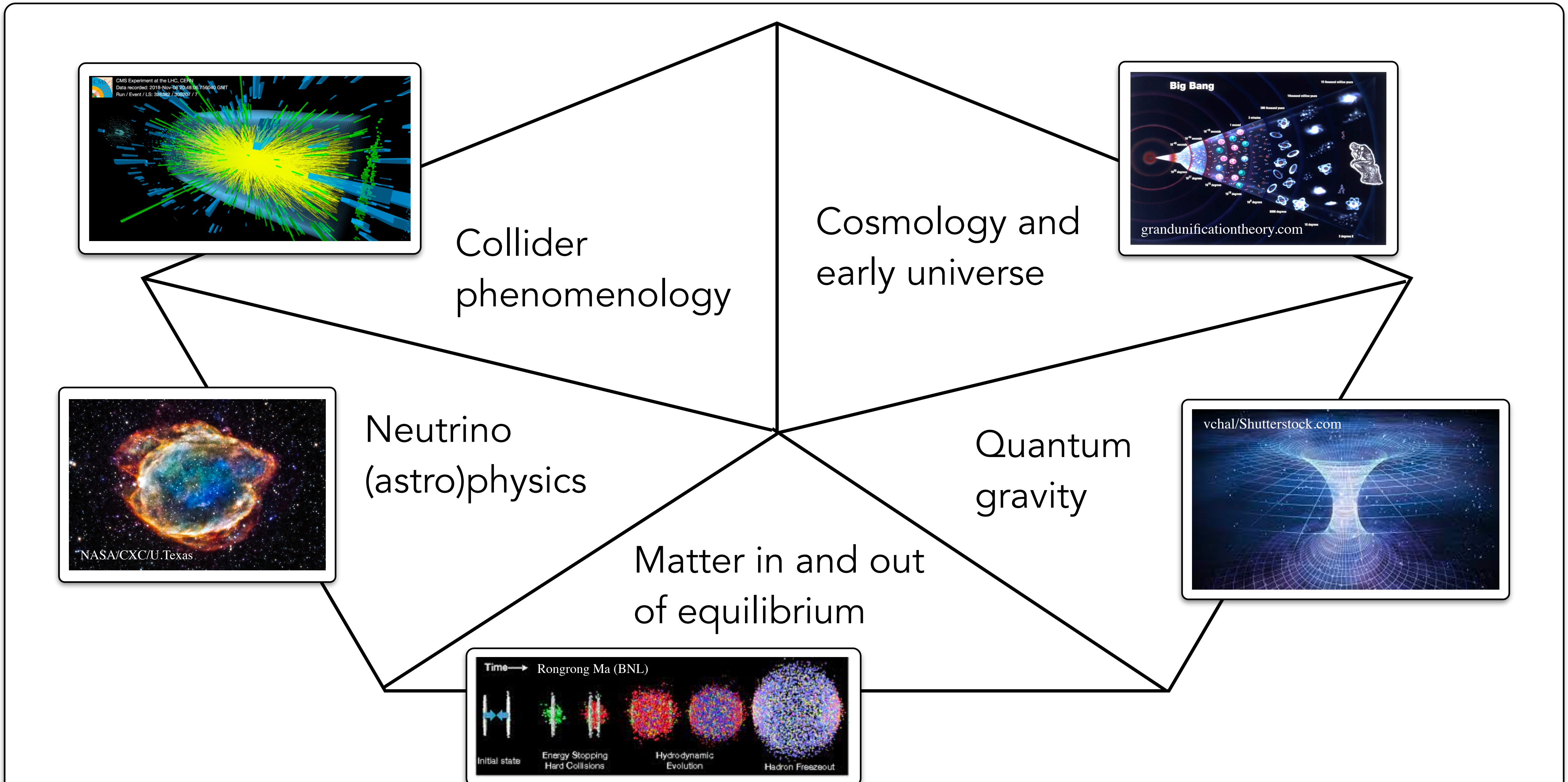
Path integral formulation:

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

Hamiltonian evolution:

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

PLUS MANY INTRACTABLE QUESTIONS IN HIGH ENERGY PHYSICS AS WELL…



Bauer, ZD, MJS et al, arXiv:2204.03381 [quant-ph].

Quantum Simulation for High-energy Physics

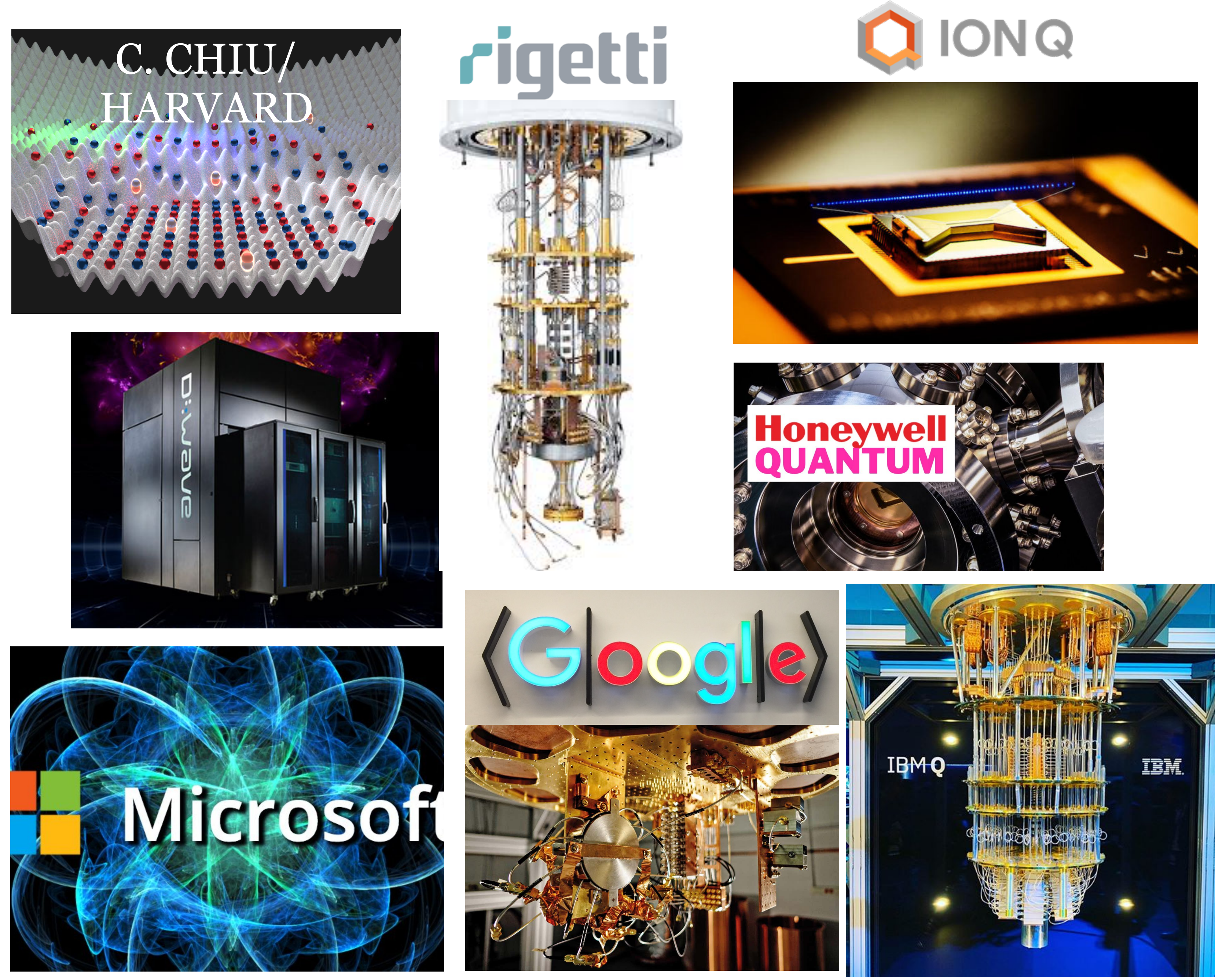
Christian Bauer,[1,a] Zohreh Davoudi,[2,b] A. Baha Balantekin,[3] Tanmoy Bhattacharya,[4] Marcela Carena,[5,6,7] Wibe A. de Jong,[1] Nate Gemelke,[8] Dmitri Kharzeev,[9] Henry Lamm,[5] Ying-Ying Li,[5] Yannick Meurice,[10] Christopher Monroe,[11,12,13,14] Benjamin Nachman,[1] Guido Pagano,[15] John Preskill,[16] Alessandro Roggero,[17,18] David I. Santiago,[19,20] Martin J. Savage,[21] Irfan Siddiqi,[19,20,22] George Siopsis,[23] Yukari Yamauchi,[2] and Kübra Yeter-Aydeniz[24]

An opportunity to explore new paradigms and new technologies:
Turning to quantum simulation

https://www.pechakucha.com/

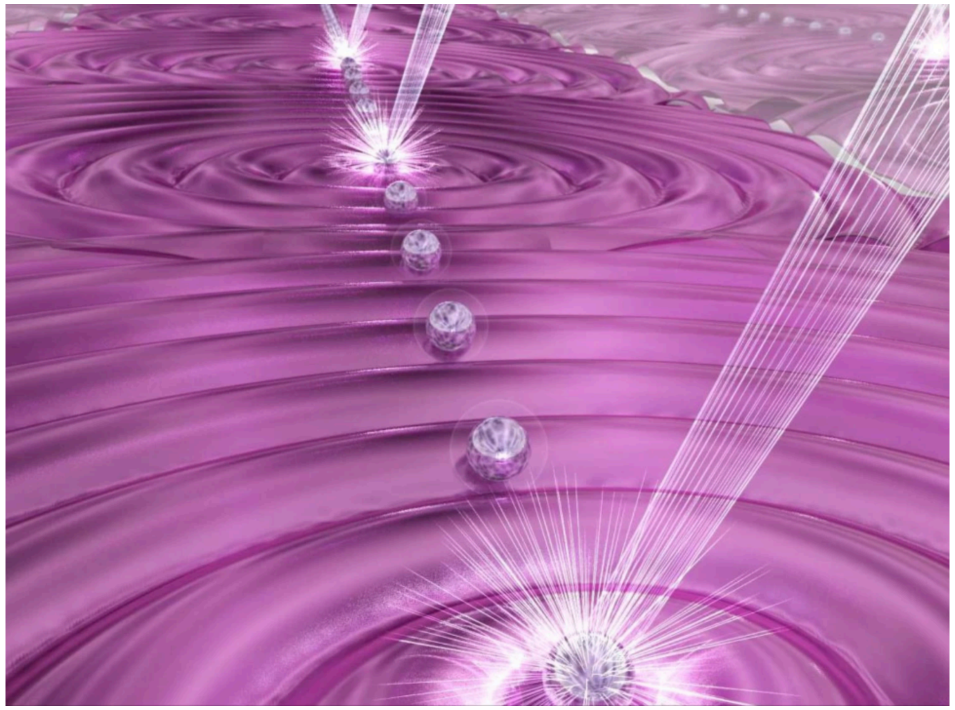
A RANGE OF QUANTUM SIMULATORS WITH VARING CAPACITY AND CAPABILITY IS AVAILABLE!

- 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)



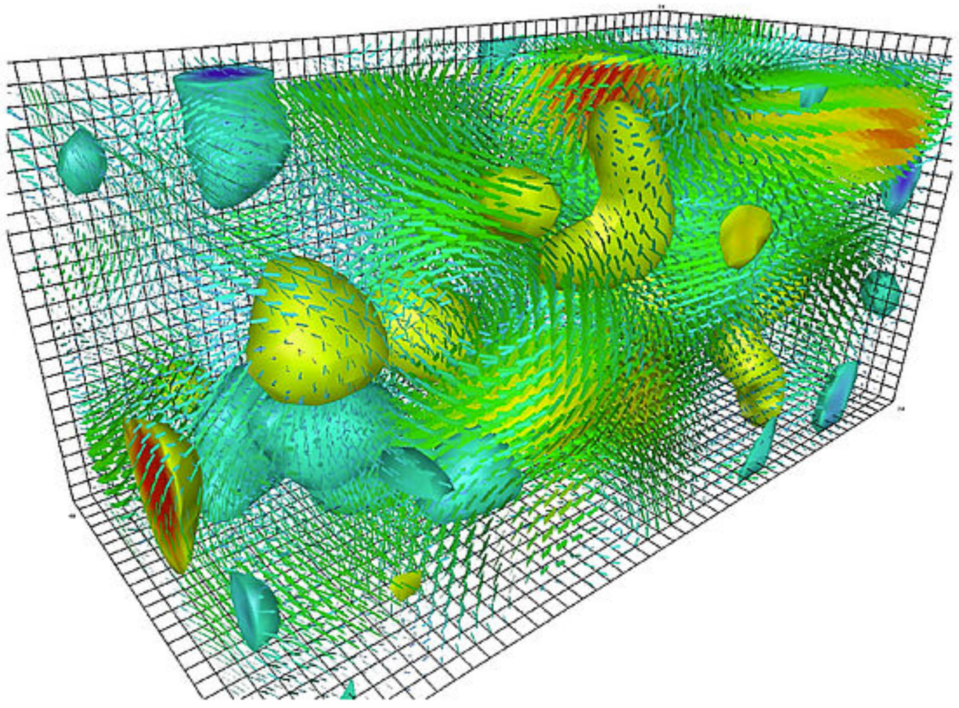
QUANTUM SIMULATION OF QCD?

A controlled quantum system



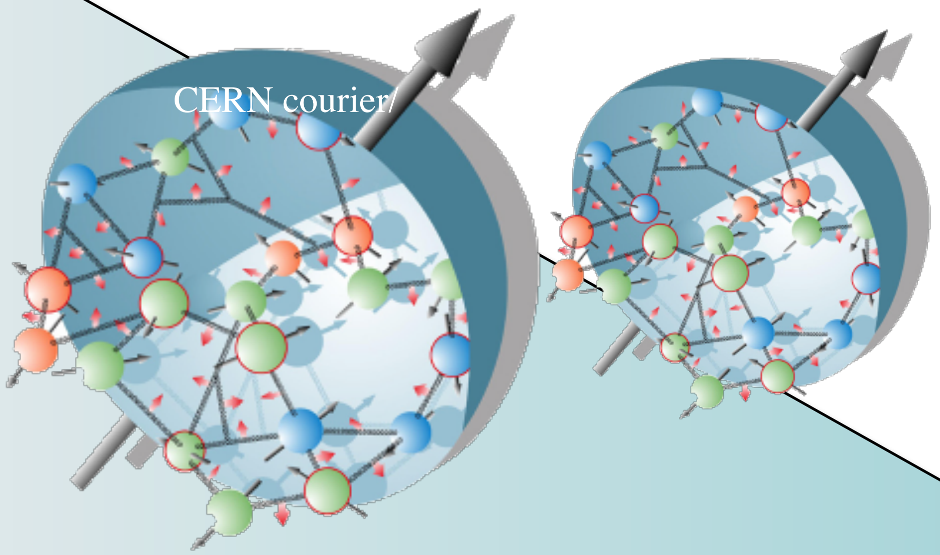
CREDIT: EMILY EDWARDS, UNIVERSITY OF MARYLAND

Strong-interaction physics



COPY RIGHT: UNIVERSITY OF ADELAIDE

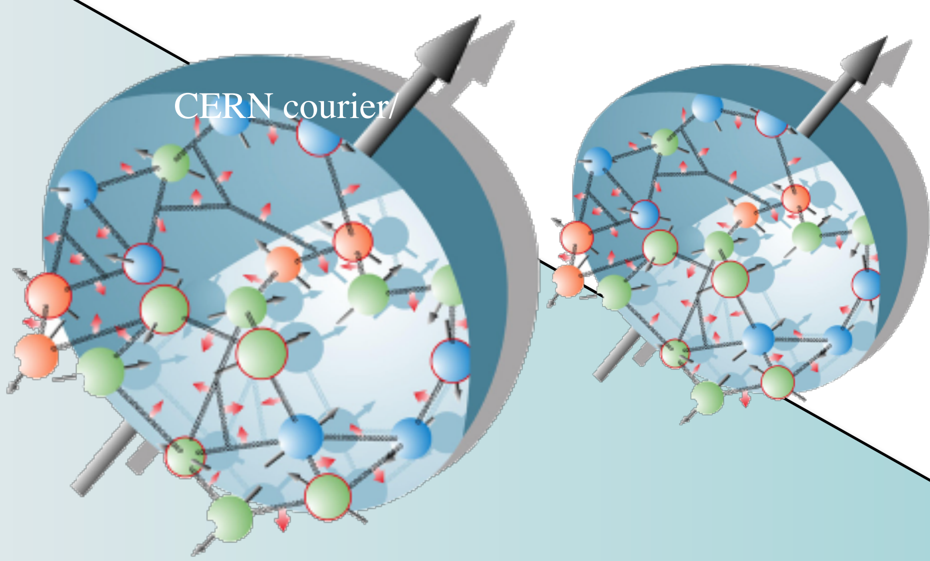
DIFFERENT FROM QUANTUM-CHEMISTRY SIMULATIONS



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.

DIFFERENT FROM QUANTUM-CHEMISTRY SIMULATIONS

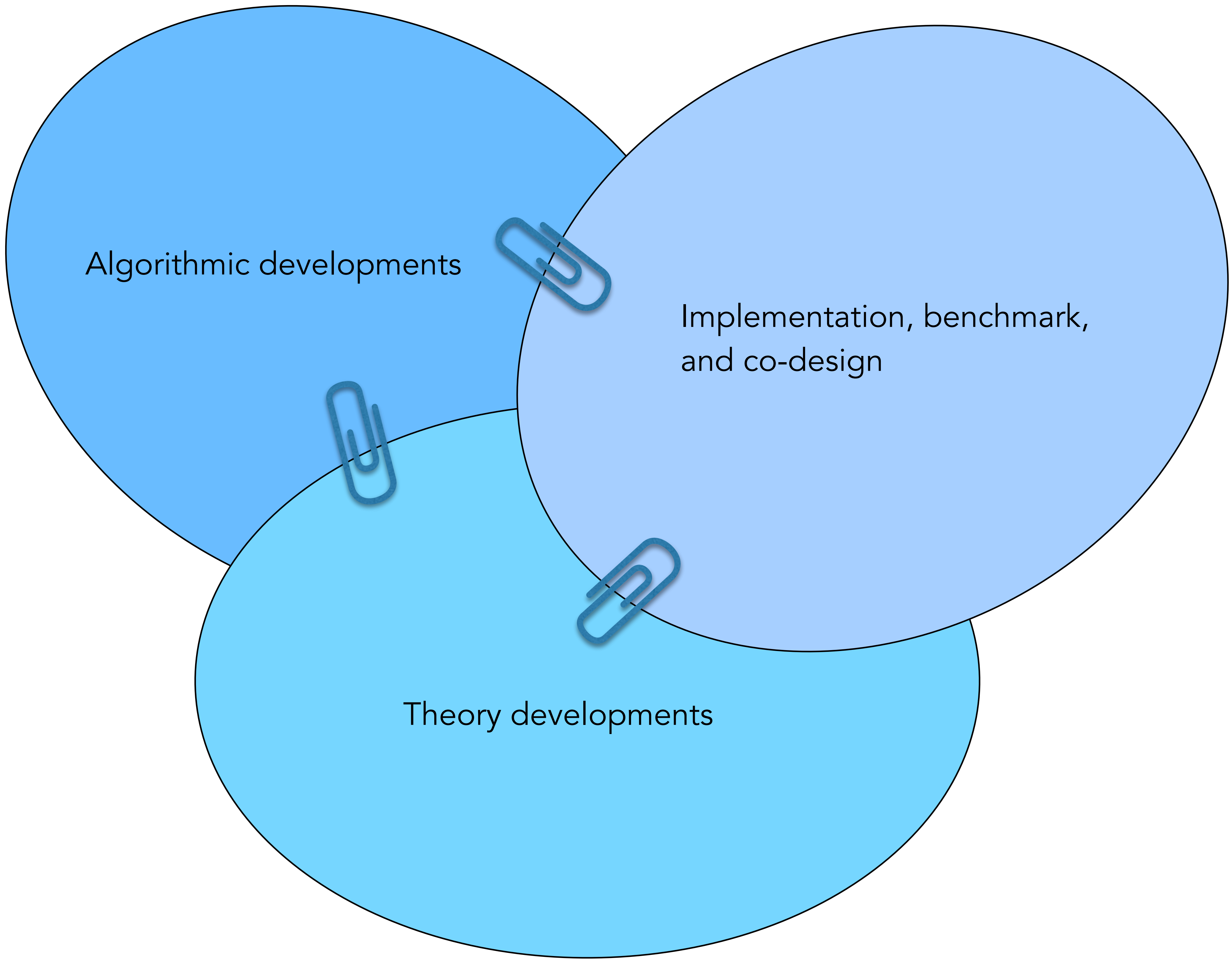


Starting from the Standard Model

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

Hamiltonian formalism maybe more natural than the path integral formalism for quantum simulation/computation:

Kogut and Susskind formulation:

$$H_{\mathrm{QCD}} = -t\sum_{\langle xy\rangle} s_{xy}\left(\psi_x^\dagger U_{xy}\psi_y + \psi_y^\dagger U_{xy}^\dagger \psi_x\right) + m\sum_x s_x \psi_x^\dagger \psi_x + \frac{g^2}{2}\sum_{\langle xy\rangle}\left(L_{xy}^2 + R_{xy}^2\right) - \frac{1}{4g^2}\sum_{\square}\mathrm{Tr}\left(U_\square + U_\square^\dagger\right).$$

Fermion hopping term

Fermion mass

Energy of color electric field

Energy of color magnetic field

QUANTUM SIMULATION OF GAUGE FIELD THEORIES: THEORY DEVELOPMENTS

Hamiltonian formalism maybe more natural than the path integral formalism for quantum simulation/computation:

Kogut and Susskind formulation:

An infinite-dimensional Hilbert space!

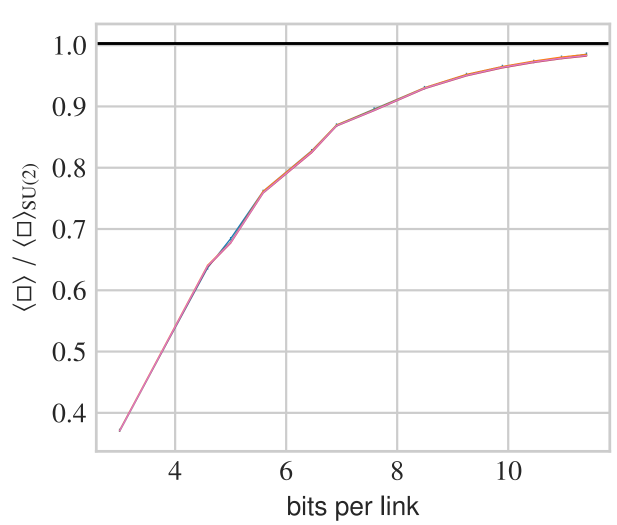
$$H_{\rm QCD} = -t\sum_{\langle xy\rangle} s_{xy}\left(\psi_x^\dagger U_{xy}\psi_y + \psi_y^\dagger U_{xy}^\dagger \psi_x\right) + m\sum_x s_x \psi_x^\dagger \psi_x + \frac{g^2}{2}\sum_{\langle xy\rangle}\left(L_{xy}^2 + R_{xy}^2\right) - \frac{1}{4g^2}\sum_{\square} {\rm Tr}\left(U_\square + U_\square^\dagger\right).$$

Fermion hopping term | Fermion mass | Energy of color electric field | Energy of color magnetic field

Tong, Albert, McClean, Preskill, and Su (2021).

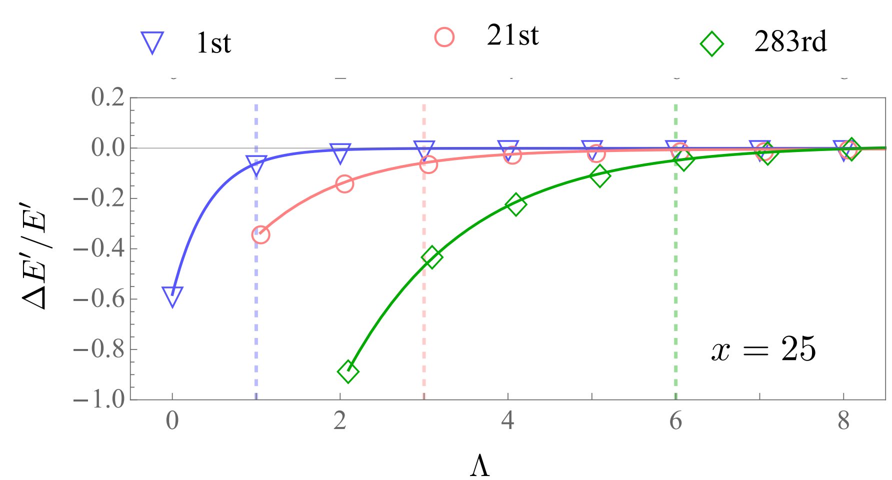
Gauge-field truncation

SU(2) pure gauge in 3+1 D in group element basis



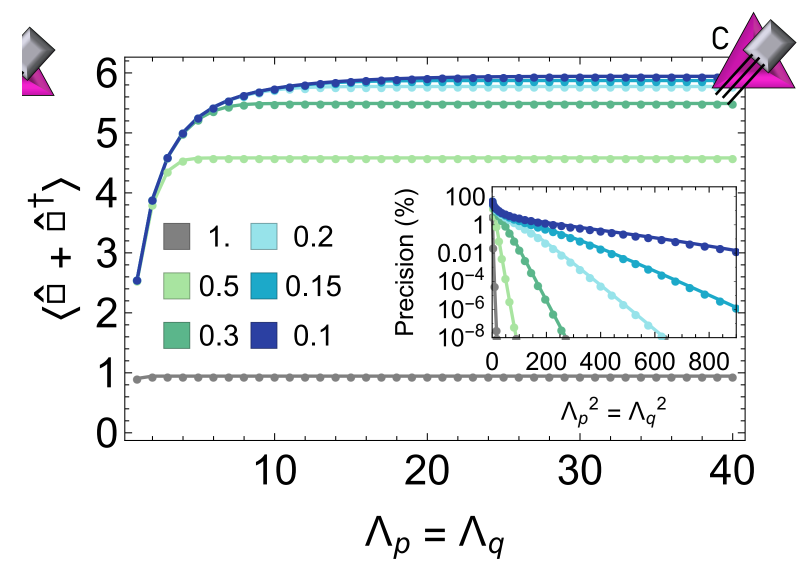
Hackett et al, Phys. Rev. A 99, 062341 (2019)

SU(2) with matter in 1+1 D in electric-field basis



ZD, Raychowdhury, and Shaw, arXiv:2009.11802 [hep-lat]

SU(3) pure gauge in 2+1 D in local-irreps basis



Ciavarella, Klco, and Savage, arXiv:2101.10227 [quant-ph]

QUANTUM SIMULATION OF GAUGE FIELD THEORIES: THEORY DEVELOPMENTS

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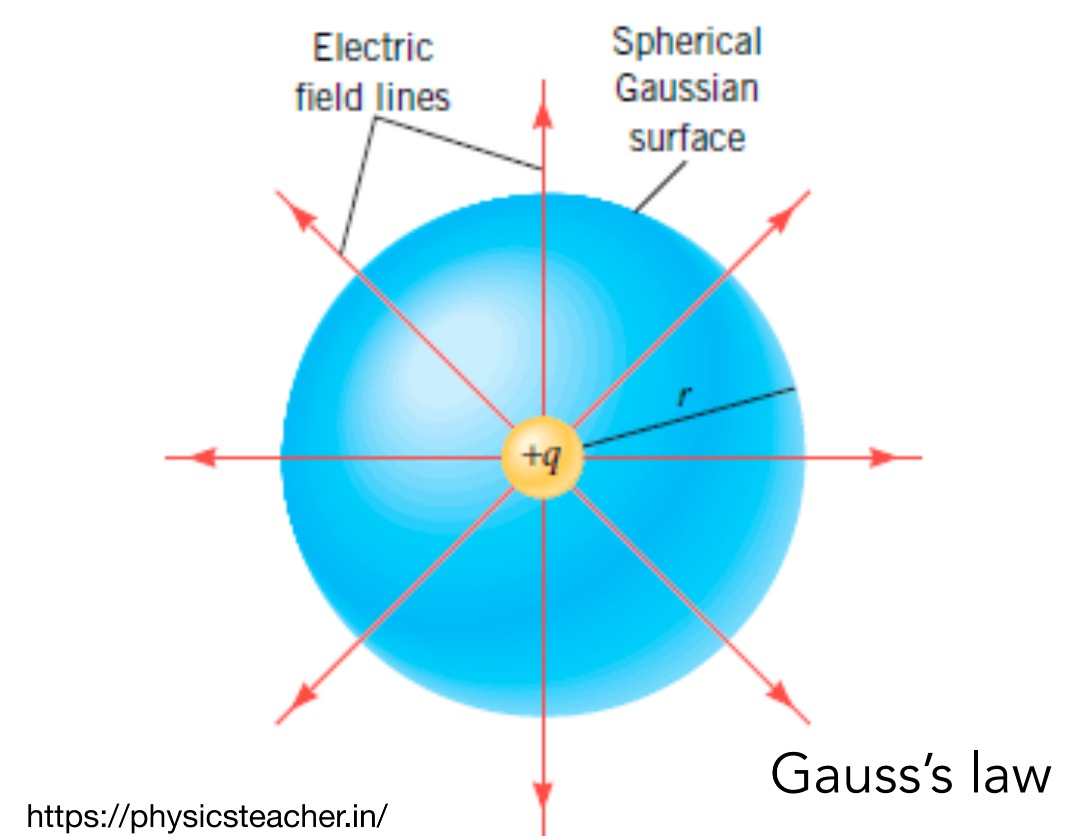
Fermion hopping term | Fermion mass | Energy of color electric field | Energy of color magnetic field

Generator of infinitesimal gauge transformation $G_x^a = \psi_x^{i\dagger}\lambda_{ij}^a\psi_x^j + \sum_k \left(L_{x,x+\hat{k}}^a + R_{x-\hat{k},x}^a\right) \Longrightarrow G_x^i|\psi(\{q_x^{(i)}\})\rangle = q_x^{(i)}|\psi(\{q_x^{(i)}\})\rangle$



Gauss's law

QUANTUM SIMULATION OF GAUGE FIELD THEORIES: THEORY DEVELOPMENTS

Hamiltonian formalism maybe more natural than the path integral formalism for quantum simulation/computation:

Kogut and Susskind formulation:

$$H_{\mathrm{QCD}} = -t\sum_{\langle xy\rangle} s_{xy}\left(\psi_x^\dagger U_{xy}\psi_y + \psi_y^\dagger U_{xy}^\dagger \psi_x\right) + m\sum_x s_x \psi_x^\dagger \psi_x + \frac{g^2}{2}\sum_{\langle xy\rangle}\left(L_{xy}^2 + R_{xy}^2\right) - \frac{1}{4g^2}\sum_{\Box}\mathrm{Tr}\left(U_\Box + U_\Box^\dagger\right).$$

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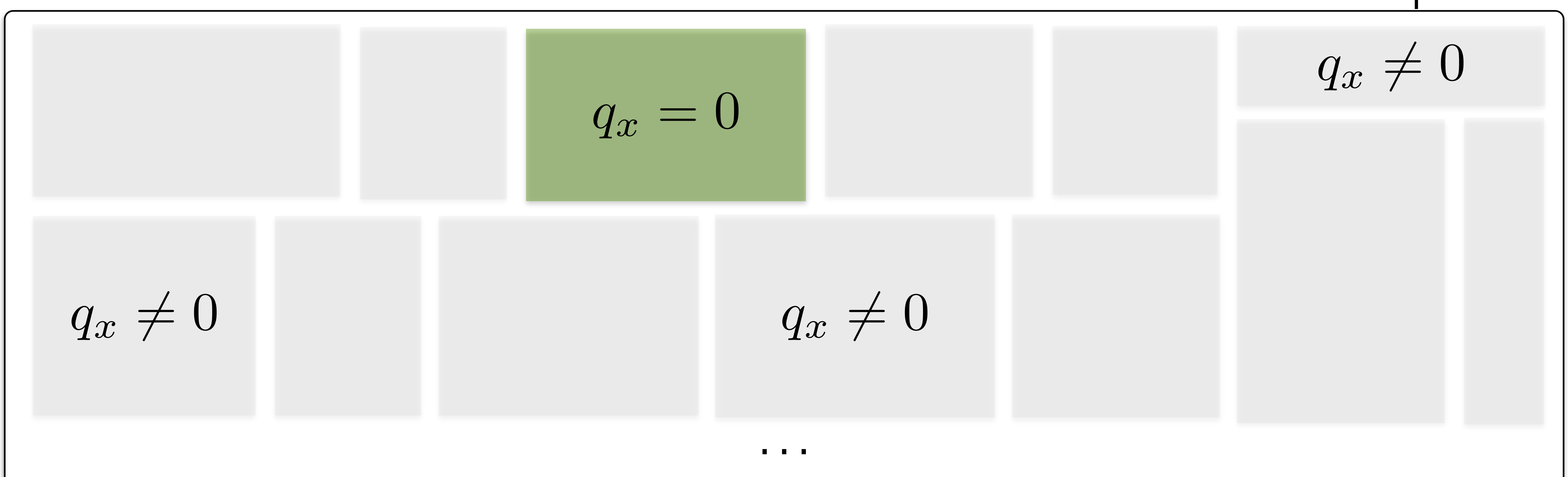
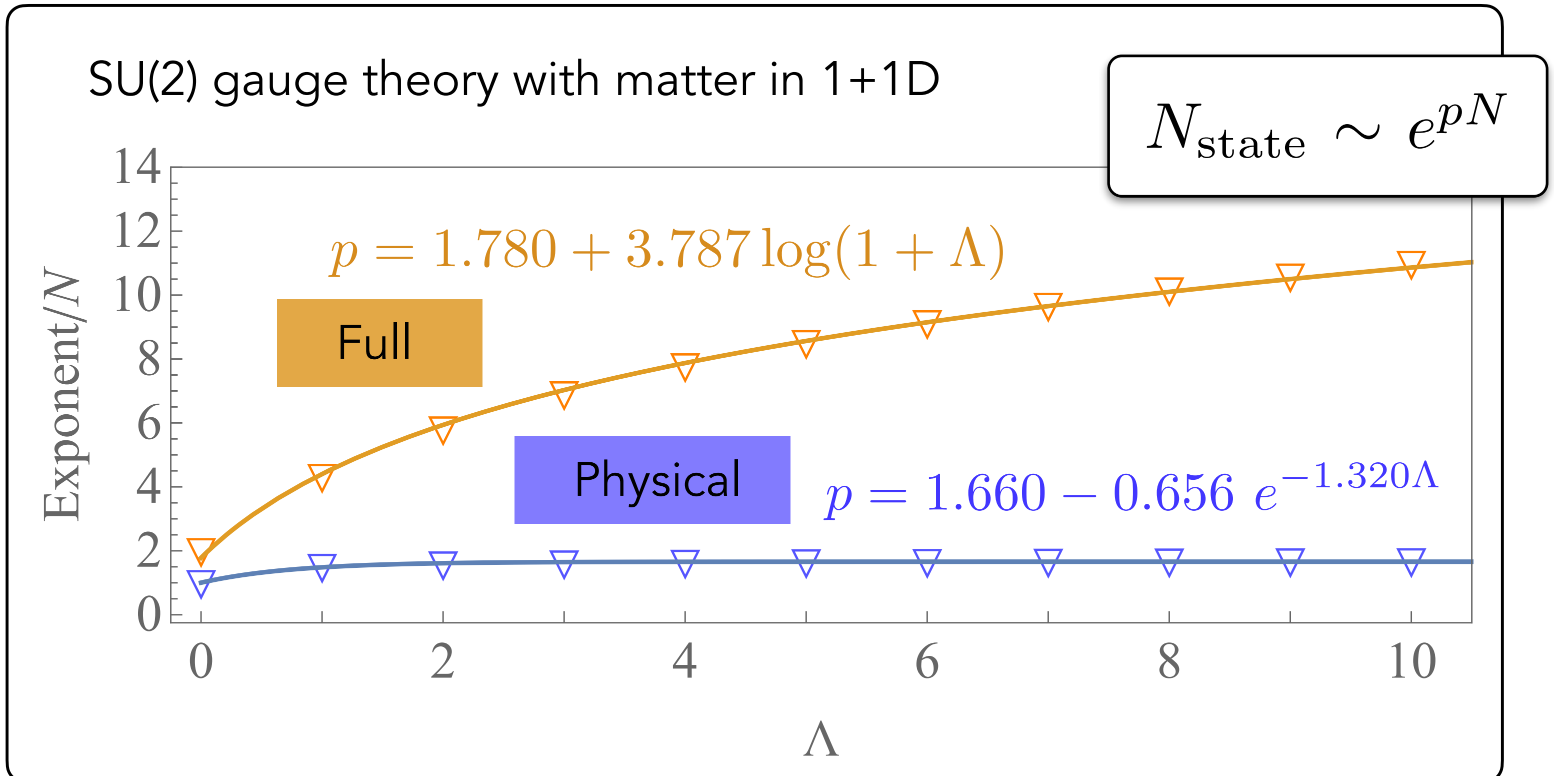
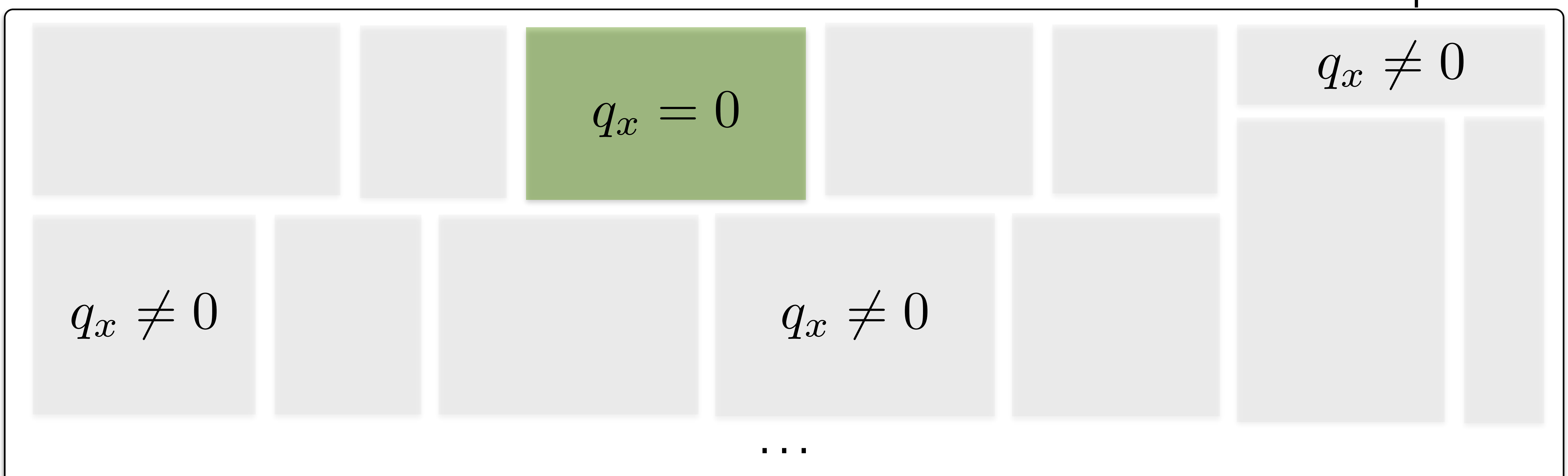


QUANTUM SIMULATION OF GAUGE FIELD THEORIES: THEORY DEVELOPMENTS



ZD, Raychowdhury, and Shaw, Phys. Rev. D 104, 074505, arXiv:2009.11802 [hep-lat]



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, ZD, Shaw

Link models
Chandrasekharan, Wiese 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.

Lots of interesting ideas using **analog simulators** will not be covered here.

Algorithmic developments [Digital]

Near- and far-term algorithms with bounded errors and resource requirement for gauge theories?

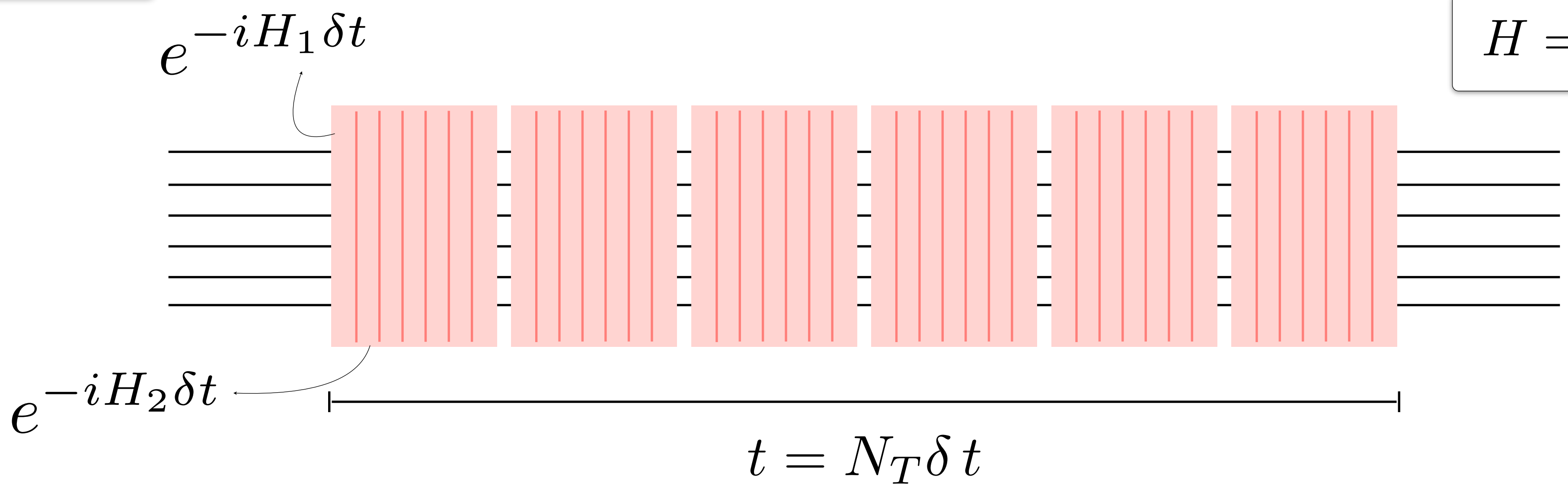
Can given formulation/encoding reduce qubit and gate resources?

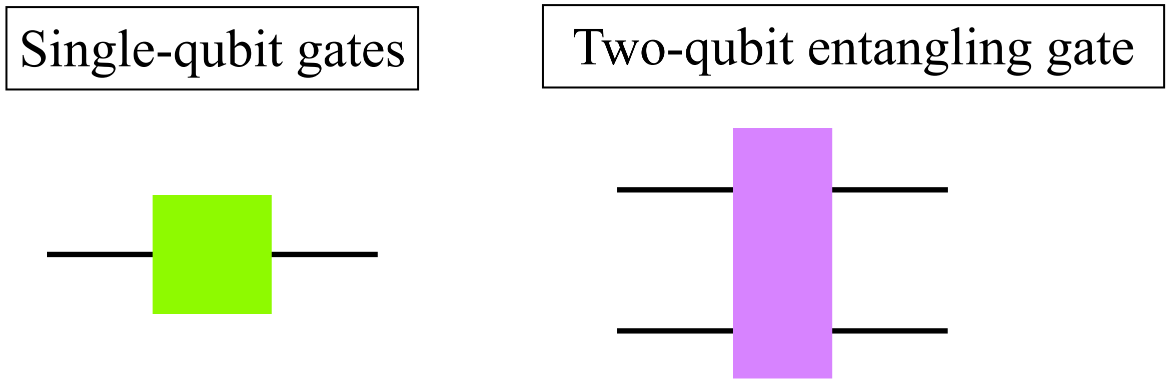
Should we develop gauge-invariant simulation algorithms?

How do we do state preparation and compute observables like scattering amplitudes?

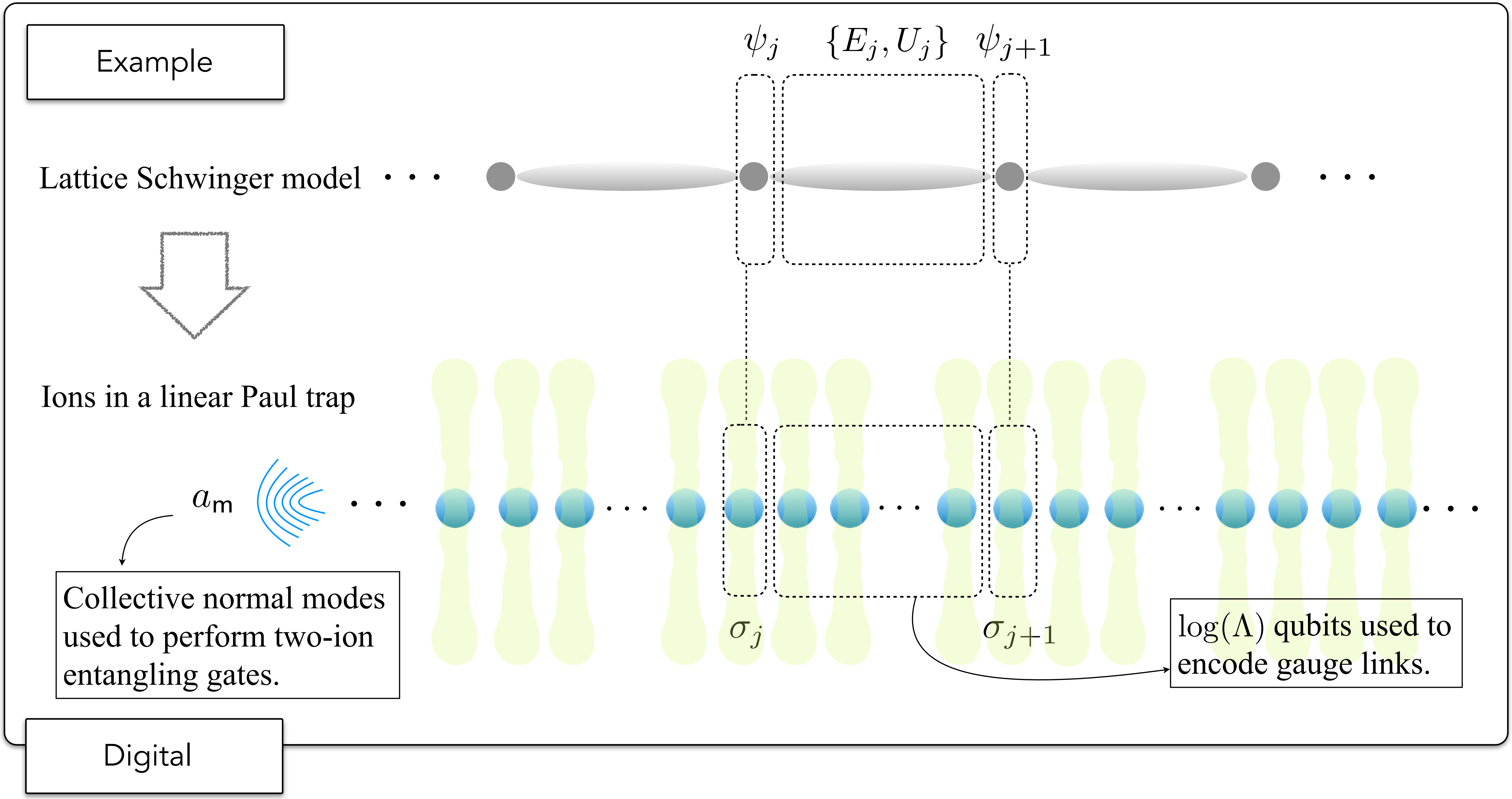
Digital

$H = H_1 + H_2 + \cdots$





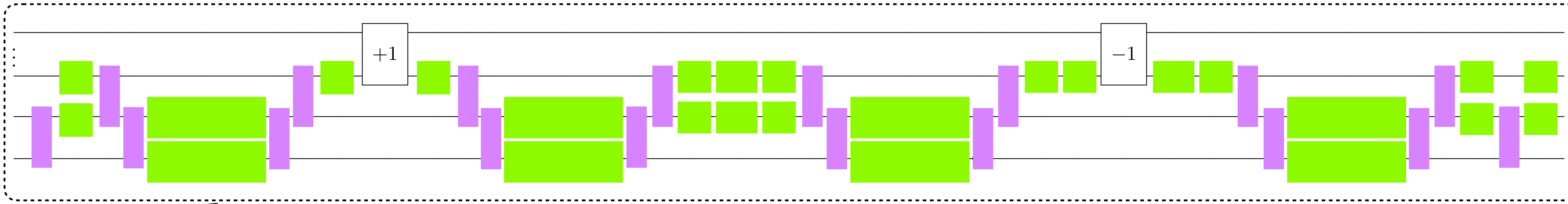
How many qubits and gates are required to achieve accuracy ϵ in a given observables? Are there algorithms that scale optimally?



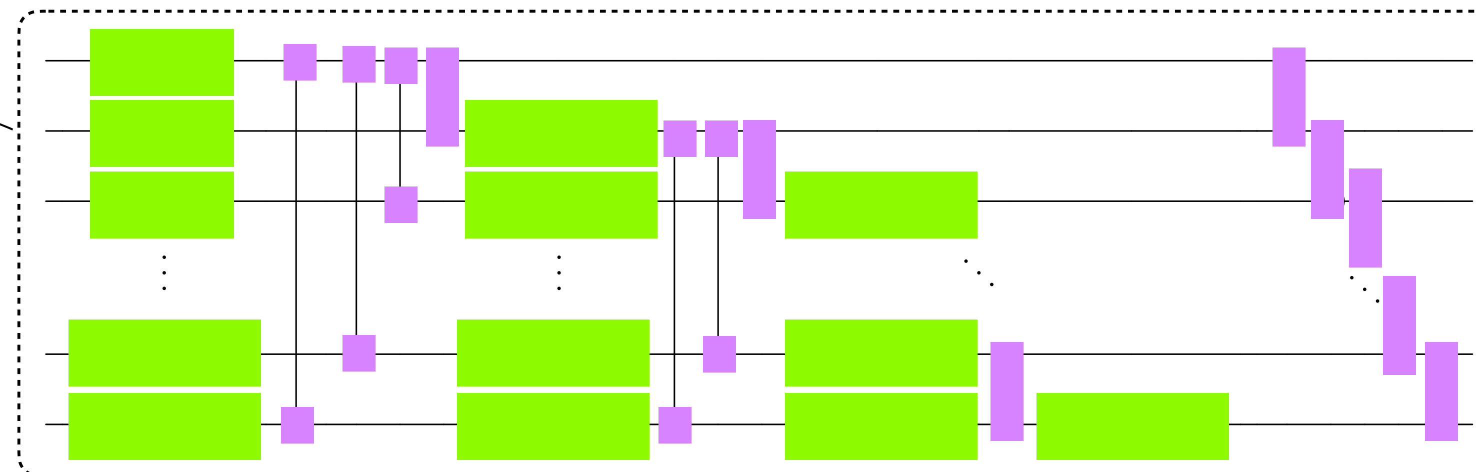
$$H = -ix \sum_{n=1}^{N-1} \left[\psi_n^\dagger U_n \psi_{n+1} - \mathrm{h.c.}\right] + \sum_{n=1}^{N-1} E_n^2 + \mu \sum_{n=1}^{N} (-1)^n \psi_n^\dagger \psi_n$$

Circuit and recourse analysis

Shaw, Lougovski, Stryker, Wiebe, Quantum 4, 306 (2020).



Sample gauge-fermion interaction block



Part of electric field interactions acting on gauge DOF registers

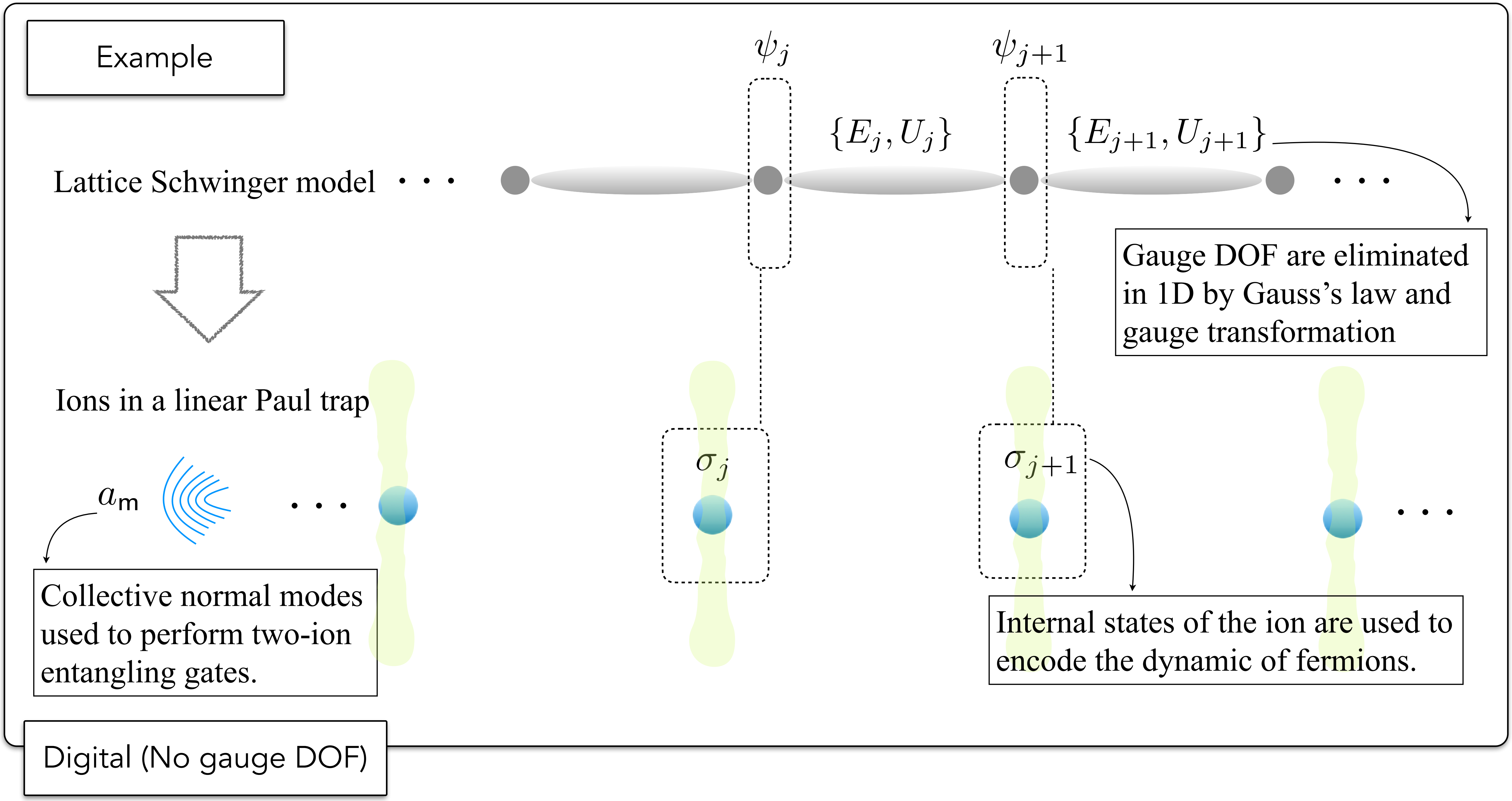
Near term cost

	$\delta_g = 10^{-3}$		$\delta_g = 10^{-4}$		$\delta_g = 10^{-5}$		$\delta_g = 10^{-6}$		$\delta_g = 10^{-7}$	
	$\tilde{\epsilon}^2$	CNOT	$\tilde{\epsilon}^2$	CNOT	$\tilde{\epsilon}^2$	CNOT	$\tilde{\epsilon}^2$	CNOT	$\tilde{\epsilon}^2$	CNOT
$x = 10^{-2}$	—	7.3e4	—	1.6e5	—	3.4e5	—	7.3e5	5.6e-2	1.6e6
$x = 10^{-1}$	—	1.6e4	—	3.5e4	—	7.5e4	5.9e-2	1.6e5	2.7e-3	3.5e5
$x = 1$	—	4.6e3	—	9.9e3	1.0e-1	2.1e4	4.7e-3	4.6e4	2.2e-4	9.9e4
$x = 10^2$	—	2.8e3	8.3e-1	6.1e3	3.8e-2	1.3e4	1.8e-3	2.8e4	8.2e-5	6.0e4

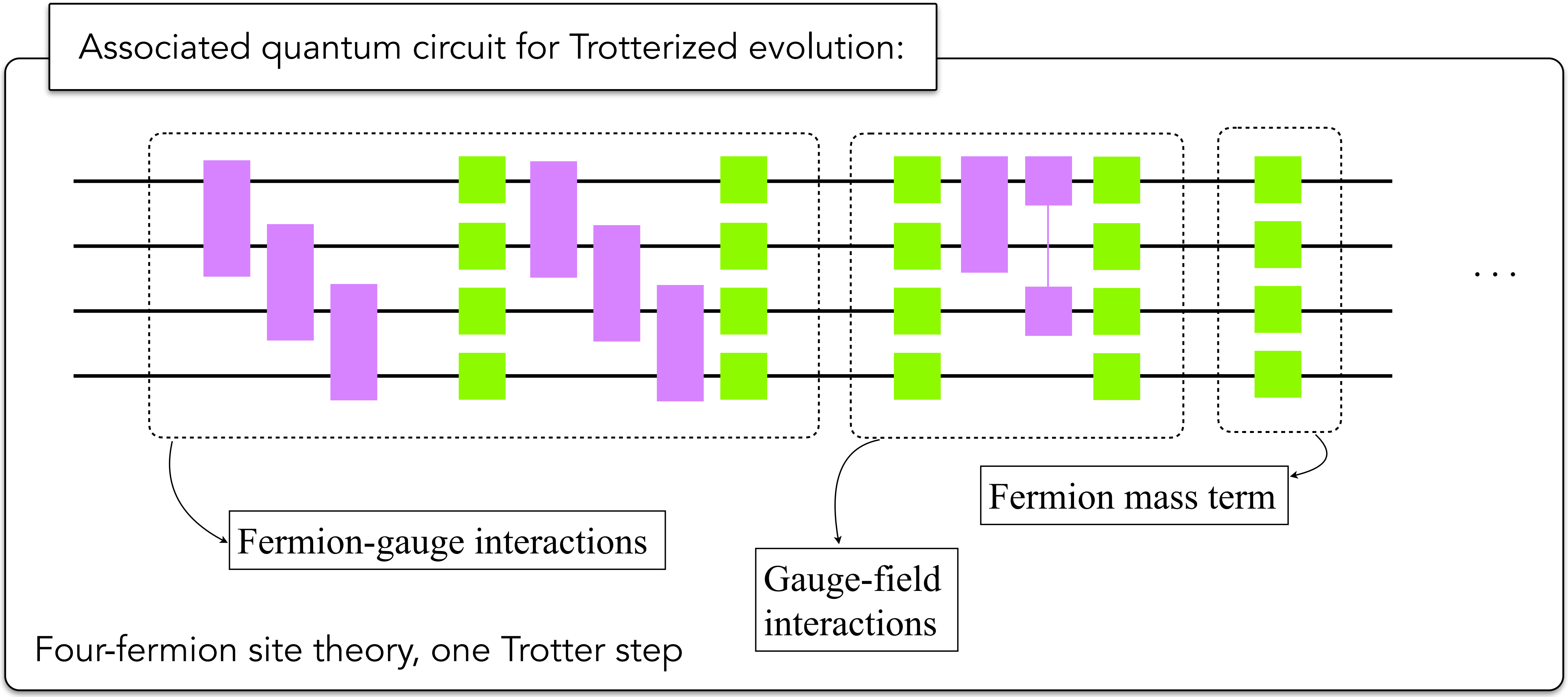
$$H = -ix \sum_{n=1}^{N-1} \left[\psi_n^\dagger U_n \psi_{n+1} - \text{h.c.}\right] + \sum_{n=1}^{N-1} E_n^2 + \mu \sum_{n=1}^{N} (-1)^n \psi_n^\dagger \psi_n$$

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?



$$H = x \sum_{n=1}^{N-1} \left[\sigma_+^{(n)} \sigma_-^{(n+1)} + \sigma_+^{(n+1)} \sigma_-^{(n)} \right] + \sum_{n=1}^{N-1} \left[\epsilon_0 + \frac{1}{2} \sum_{m=1}^{n} \left(\sigma_z^{(m)} + (-1)^m \right) \right]^2 + \frac{\mu}{2} \sum_{n=1}^{N} (-1)^n \sigma_z^{(n)}$$



$$H = x\sum_{n=1}^{N-1}\left[\sigma_+^{(n)}\sigma_-^{(n+1)} + \sigma_+^{(n+1)}\sigma_-^{(n)}\right] + \sum_{n=1}^{N-1}\left[\epsilon_0 + \frac{1}{2}\sum_{m=1}^{n}\left(\sigma_z^{(m)} + (-1)^m\right)\right]^2 + \frac{\mu}{2}\sum_{n=1}^{N}(-1)^n\sigma_z^{(n)}$$

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

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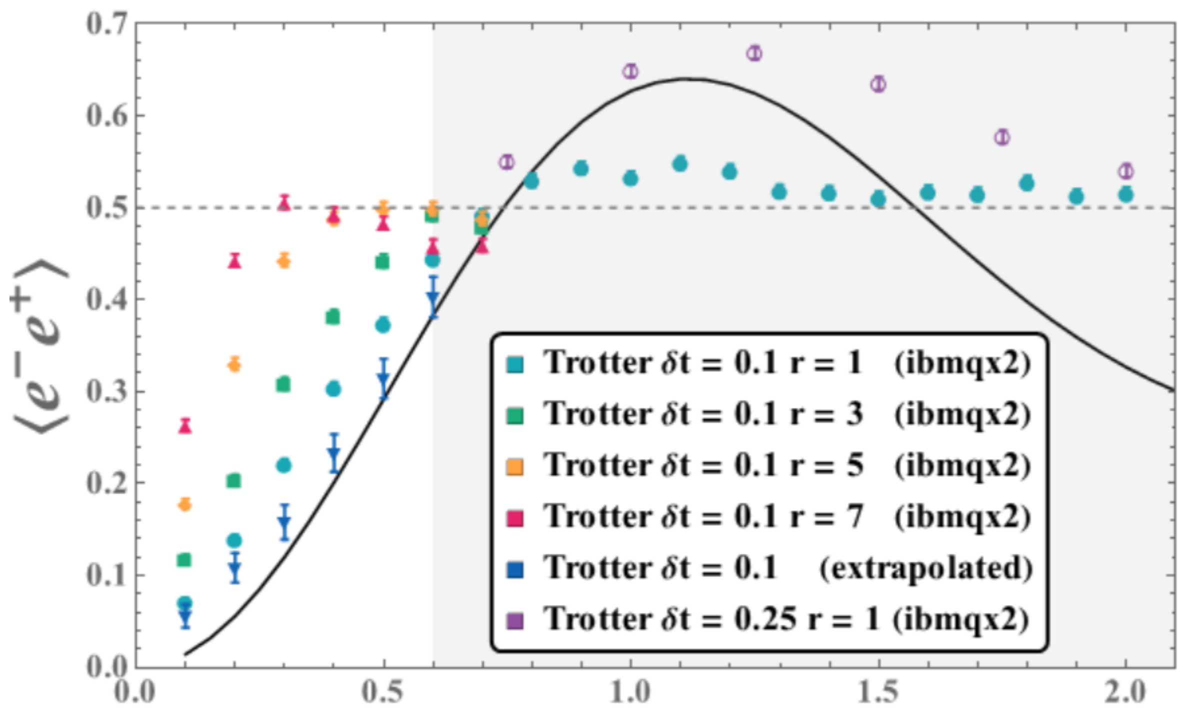

Not the spin formulation: a 2-qubit reduction of 4-qubit simulation.

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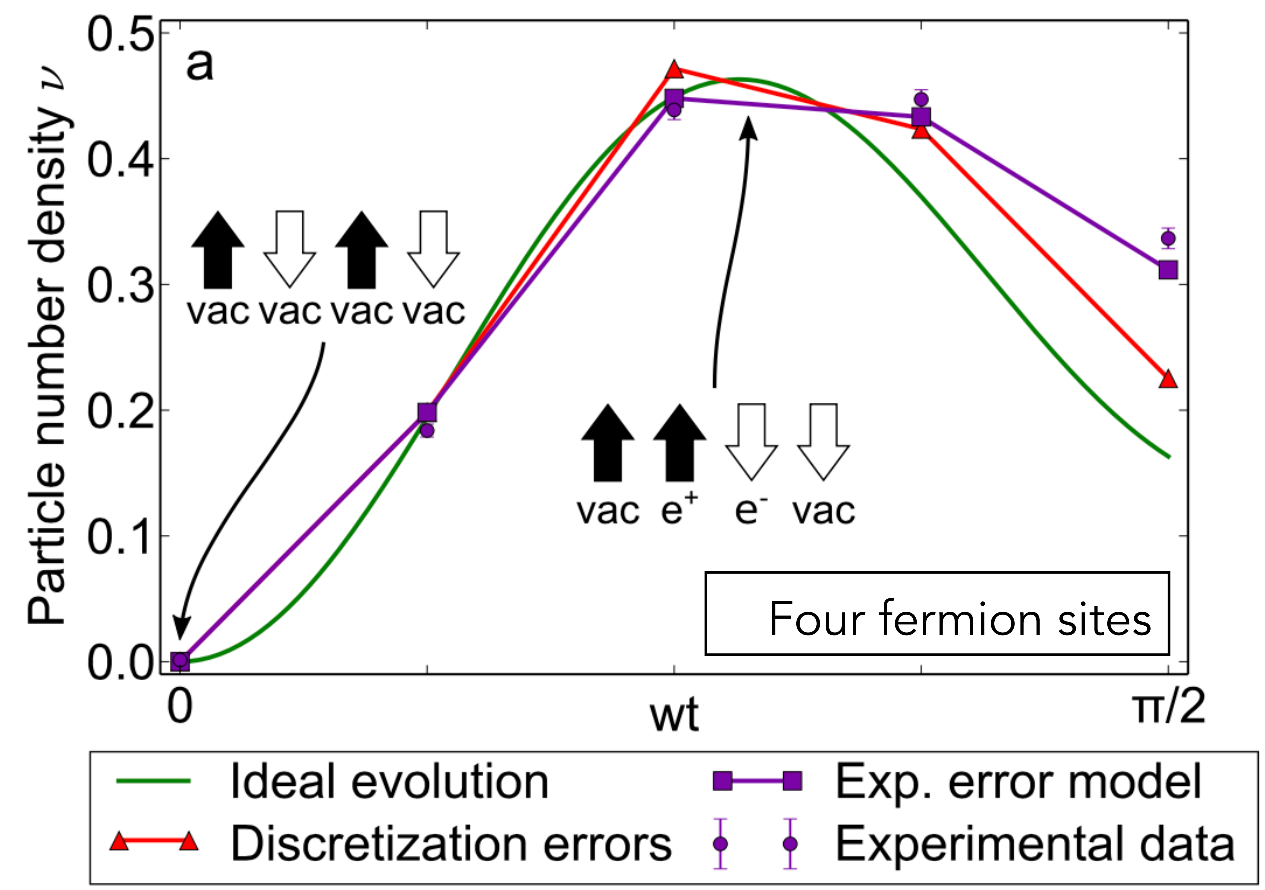
Martinez et al, Nature 534, 516 EP (2016).



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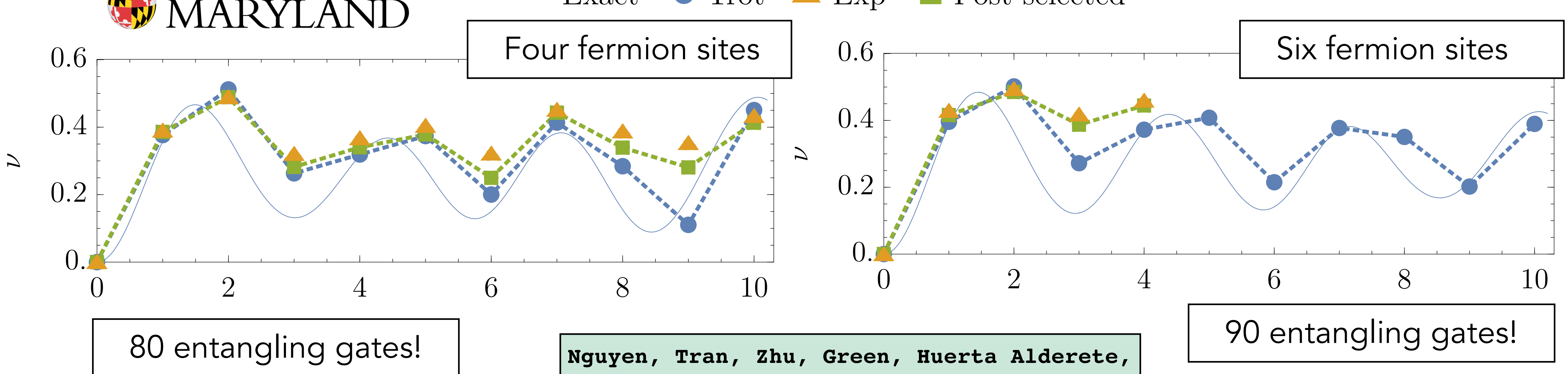
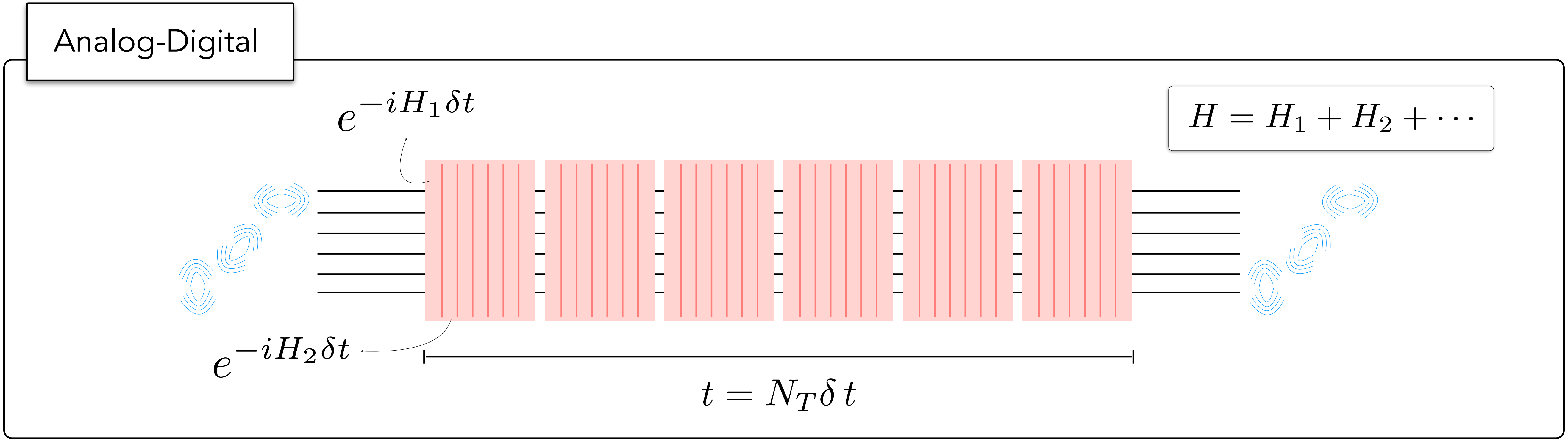
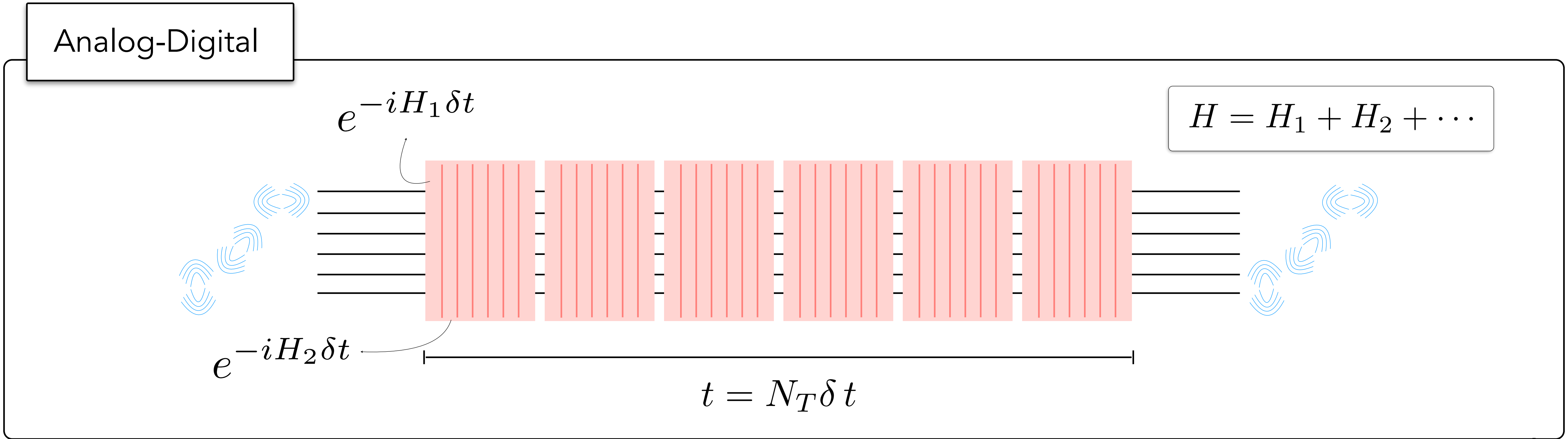
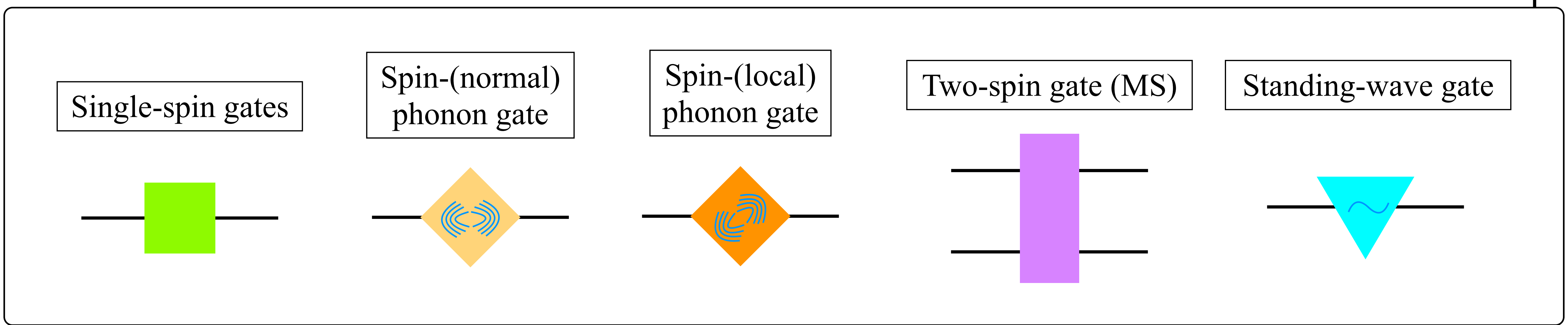


Nguyen, Tran, Zhu, Green, Huerta Alderete, ZD, Linke, *PRX Quantum* 3 (2022) 2, 020324.



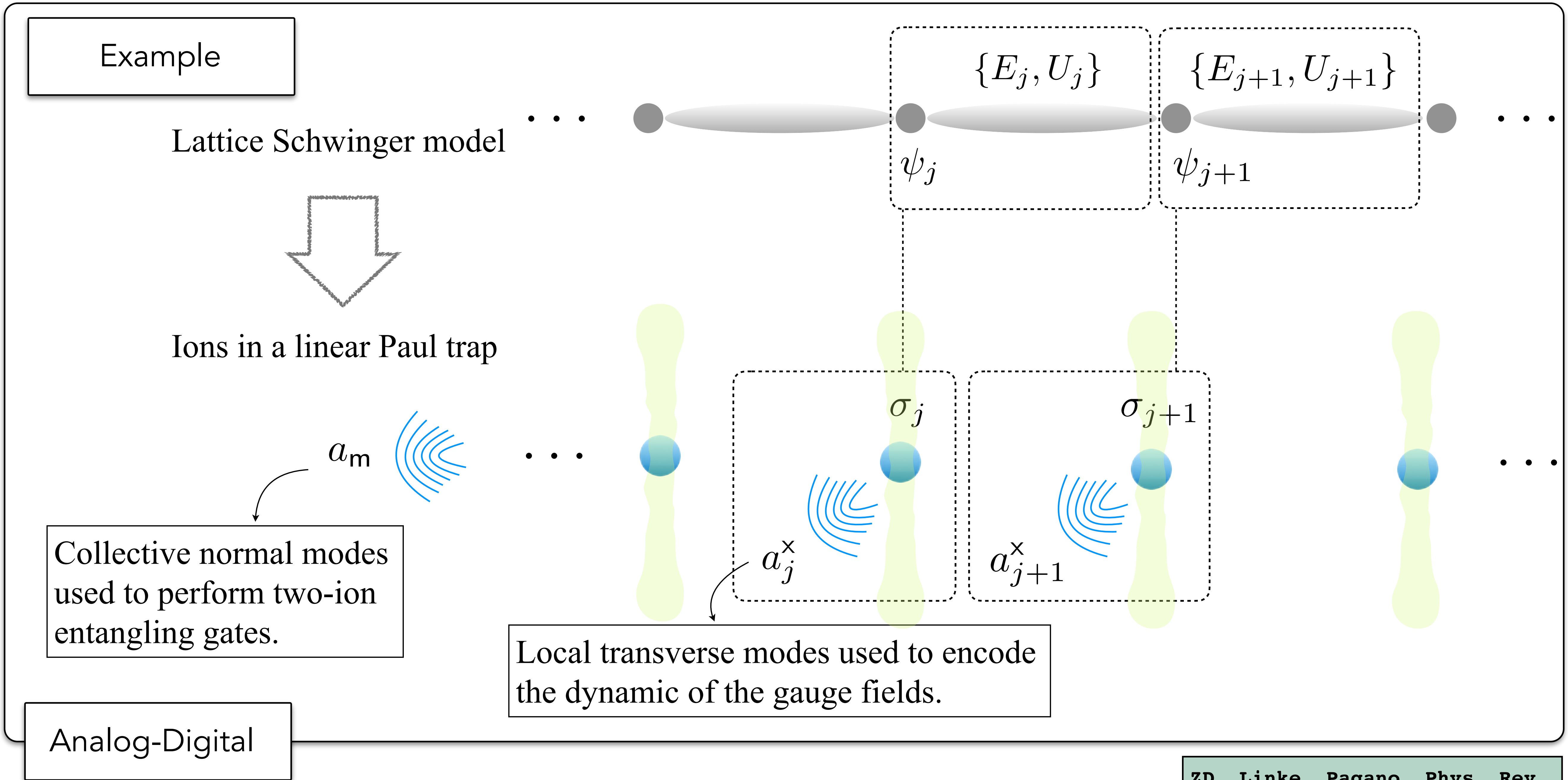
Analog-Digital
$e^{-iH_1\delta t}$
$H = H_1 + H_2 + \cdots$
$e^{-iH_2\delta t}$
$t = N_T\delta t$





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

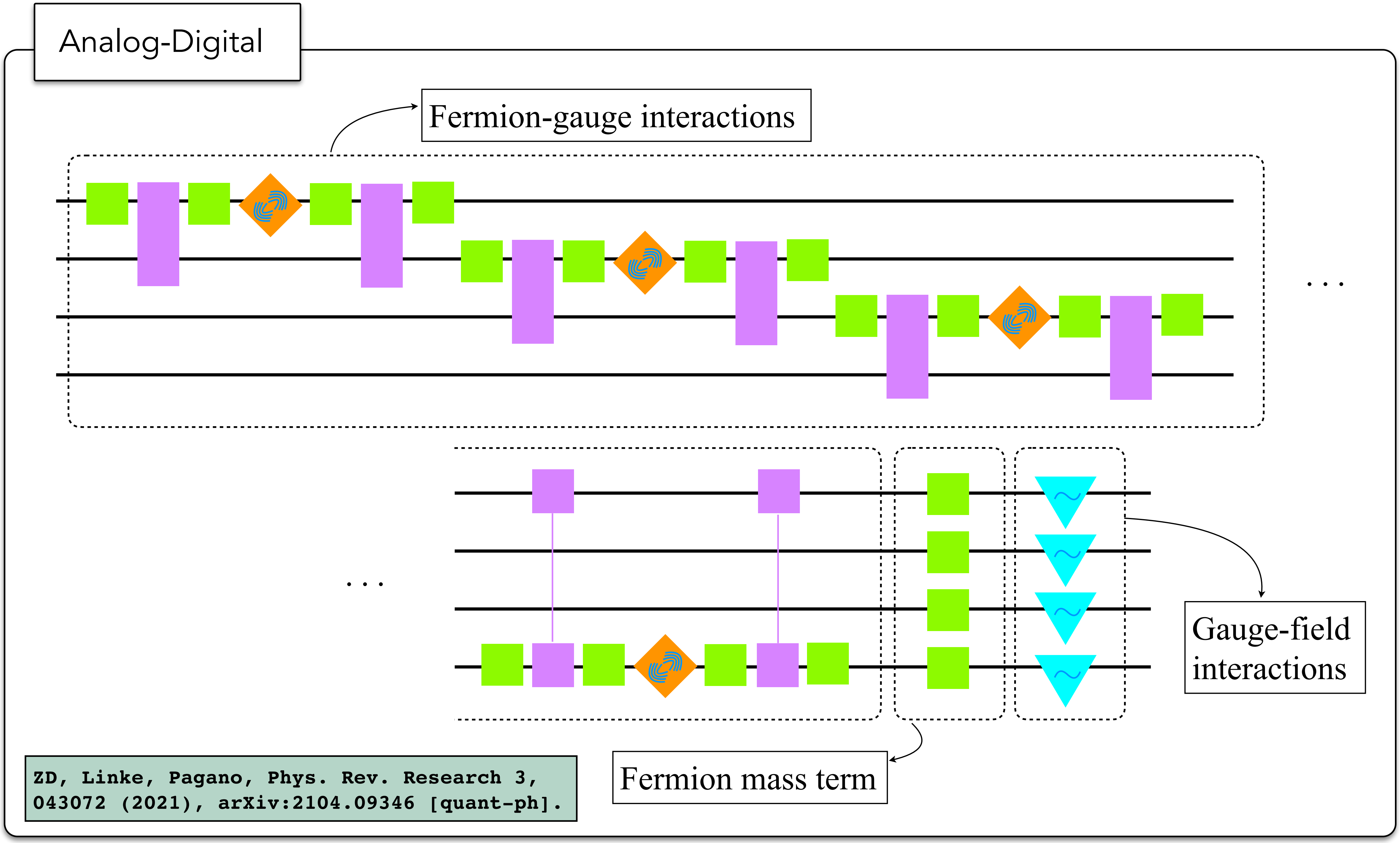
How many qubits and gates are required to achieve accuracy ϵ in a given observables? Are there algorithms that scale optimally?



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

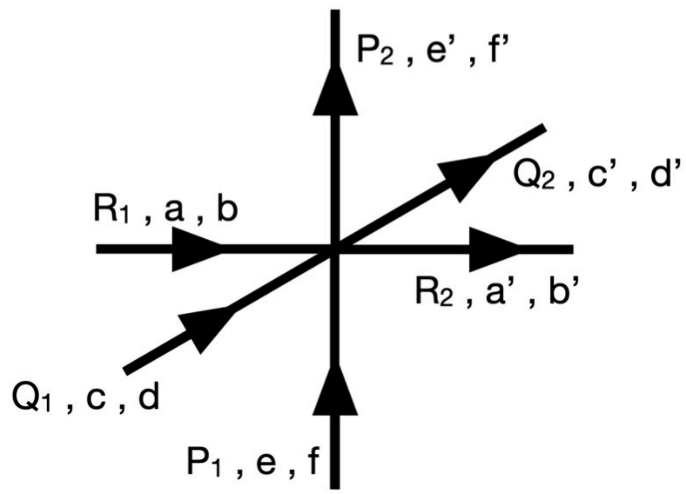
See also Casanova et al, Phys. Rev. Lett. 108, 190502 (2012), Lamata et al, EPJ Quant. Technol. 1, 9 (2014), and Mezzacapo et al, Phys. Rev. lett. 109, 200501 (2012) for analog-digital approaches to other interacting fermion-boson theories.

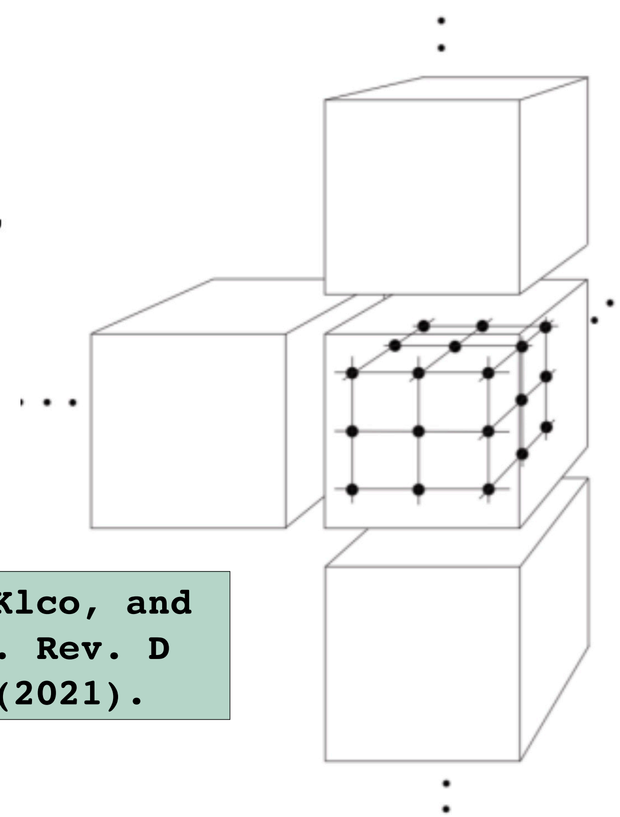
$$H = -ix \sum_{n=1}^{N-1} \left[\psi_n^\dagger U_n \psi_{n+1} - \text{h.c.}\right] + \sum_{n=1}^{N-1} E_n^2 + \mu \sum_{n=1}^{N} (-1)^n \psi_n^\dagger \psi_n$$



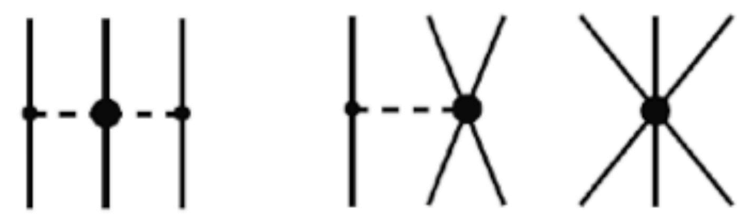
$$H = -ix \sum_{n=1}^{N-1} \left[\psi_n^\dagger U_n \psi_{n+1} - \text{h.c.}\right] + \sum_{n=1}^{N-1} E_n^2 + \mu \sum_{n=1}^{N} (-1)^n \psi_n^\dagger \psi_n$$

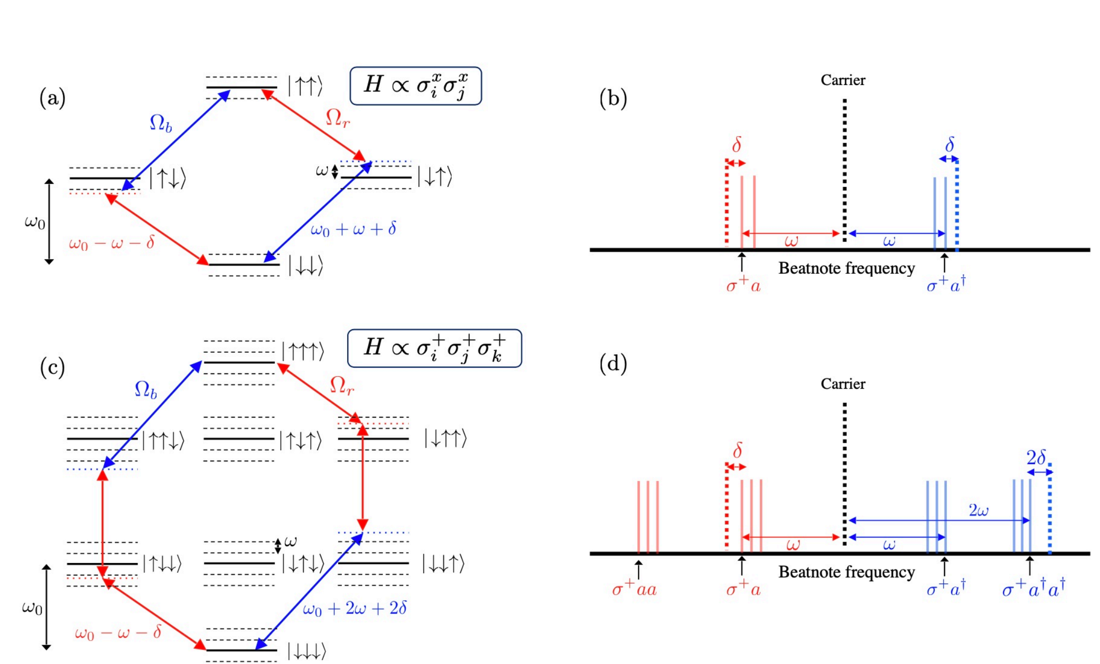
More co-design examples: Multi-dimensional local Hilbert spaces and multi-mode interactions

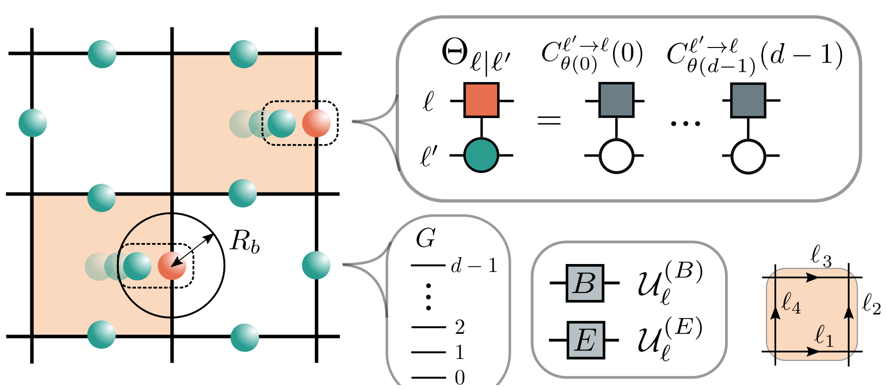




Ciavarella, Klco, and Savage, Phys. Rev. D 103, 094501 (2021).





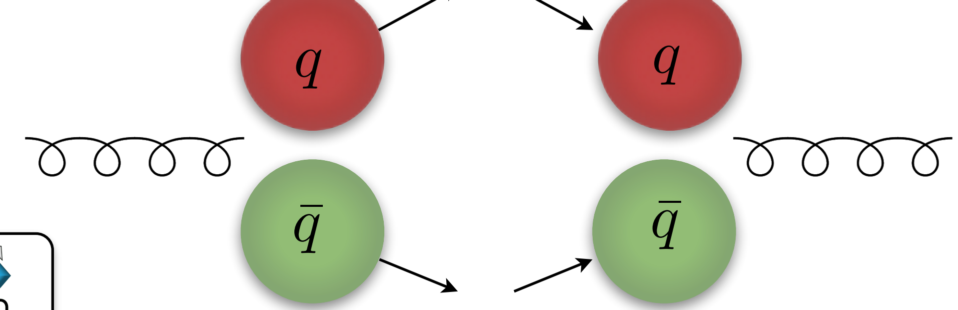


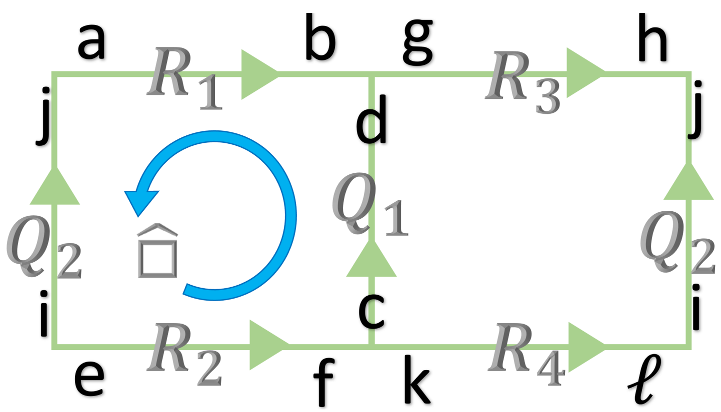
González-Cuadra, Zache, Carrasco, Kraus, Zoller, arXiv:2203.15541 [quant-ph].

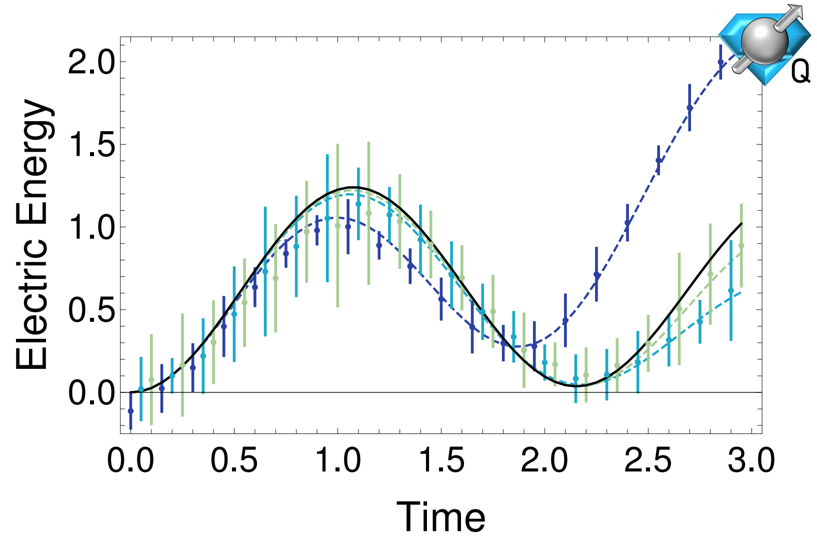
Andrade, ZD, Grass, Hafezi, Pagano, Seif, arXiv:2108.01022 [quant-ph], Bermudez et al, Pays.Rev.A79, 060303 R (2009), Katz, Centina, Monroe, arXiv:2202.04230 [quant-ph].

Finally a few more examples showcasing progress in hardware implementation of a range of QCD-inspired problems…

DIGITAL COMPUTATIONS OF NON-ABELIAN LGTs



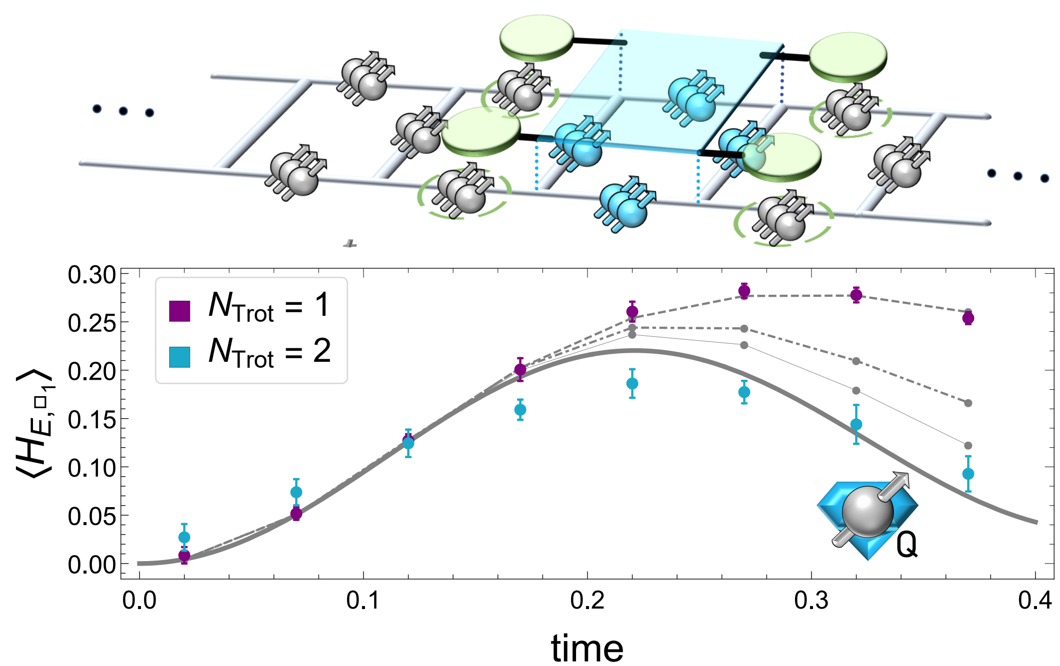




Real-time dynamic of pure SU(3) with global irrupts on IBM

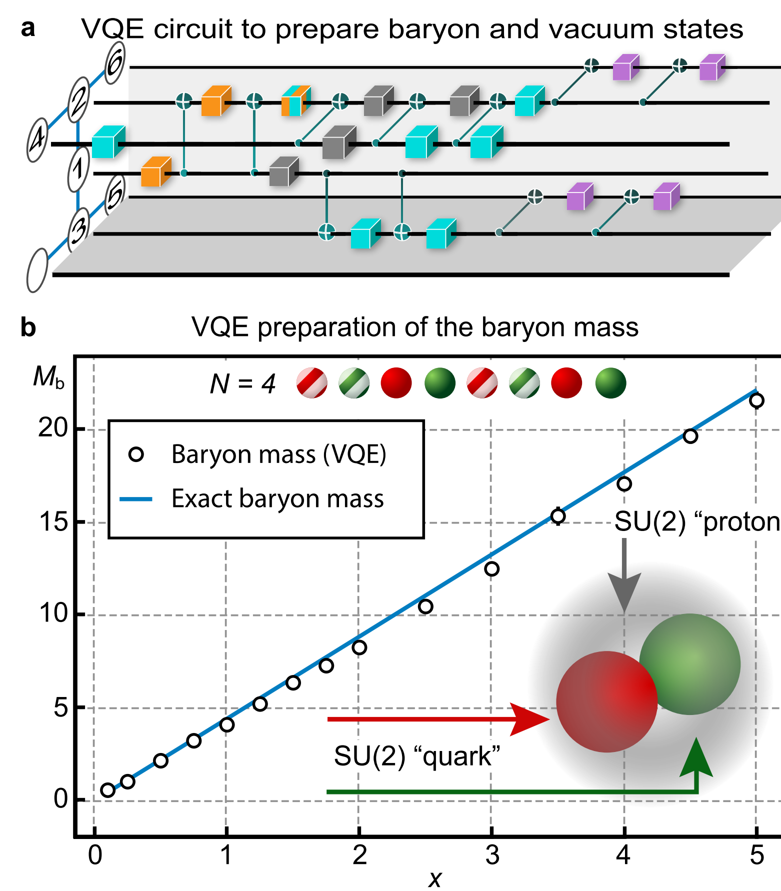
Ciavarella, Klco, and Savage, Phys. Rev. D 103, 094501 (2021).

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



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

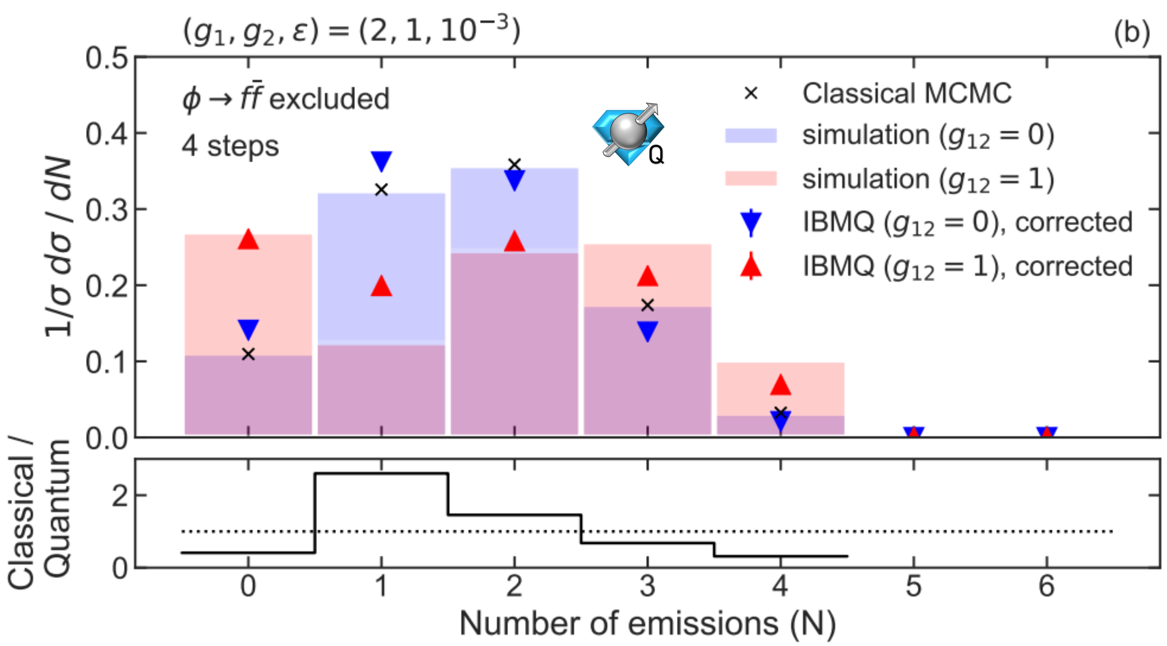
Low-lying spectrum of SU(2) with matter in 1+1 D on IBM



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

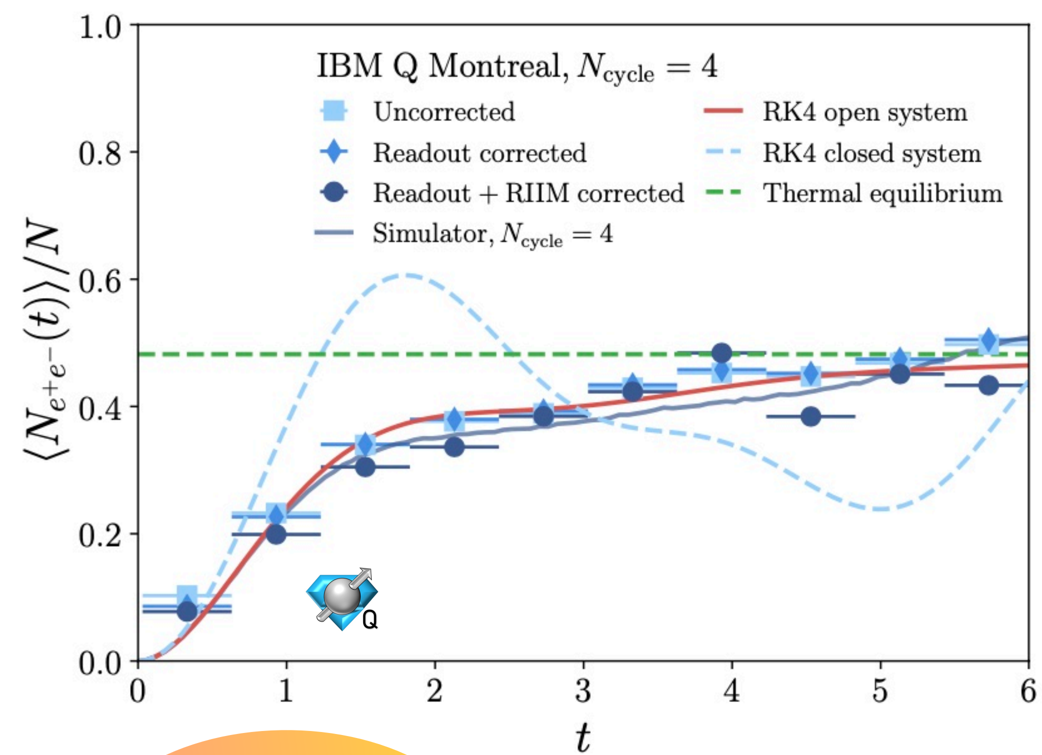
See also studies on D-wave annealers: Rahman et al, Phys. Rev. D 104, 034501 (2021), Illa and Savage, arXiv:2202.12340 [quant-ph], Farrel et al, arXiv:2207.01731 [quant-ph].

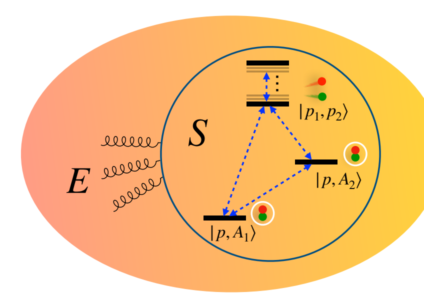
PARTON SHOWER ALGORITHMS AND HEAVY QUARKONIA MOTION IN QGP?



A polynomial time quantum final state shower algorithm that accurately models the effects of intermediate spin states similar to those present in electroweak showers.

Nachman, Provasoli, and Bauer‡, *Phys. Rev. Lett.* 126 (2021) 6, 062001.

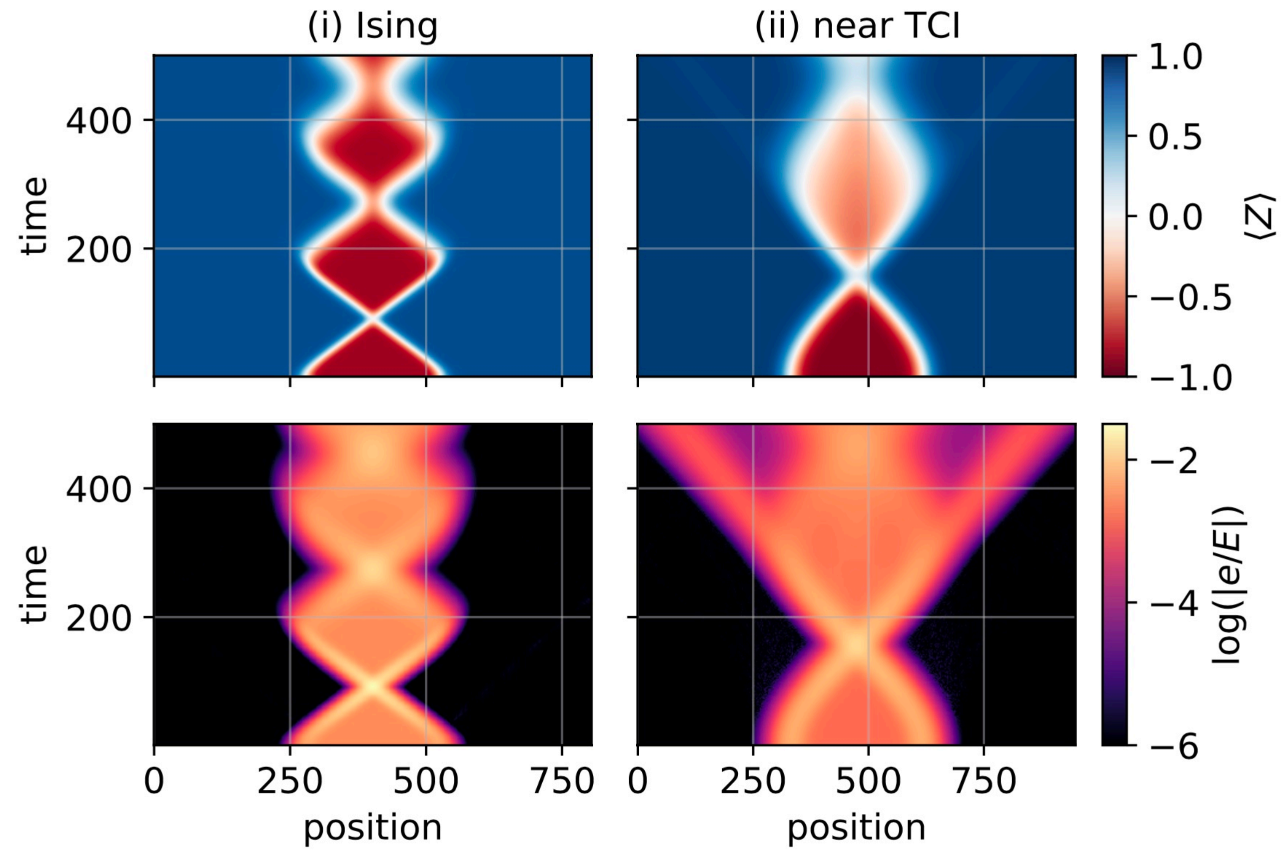




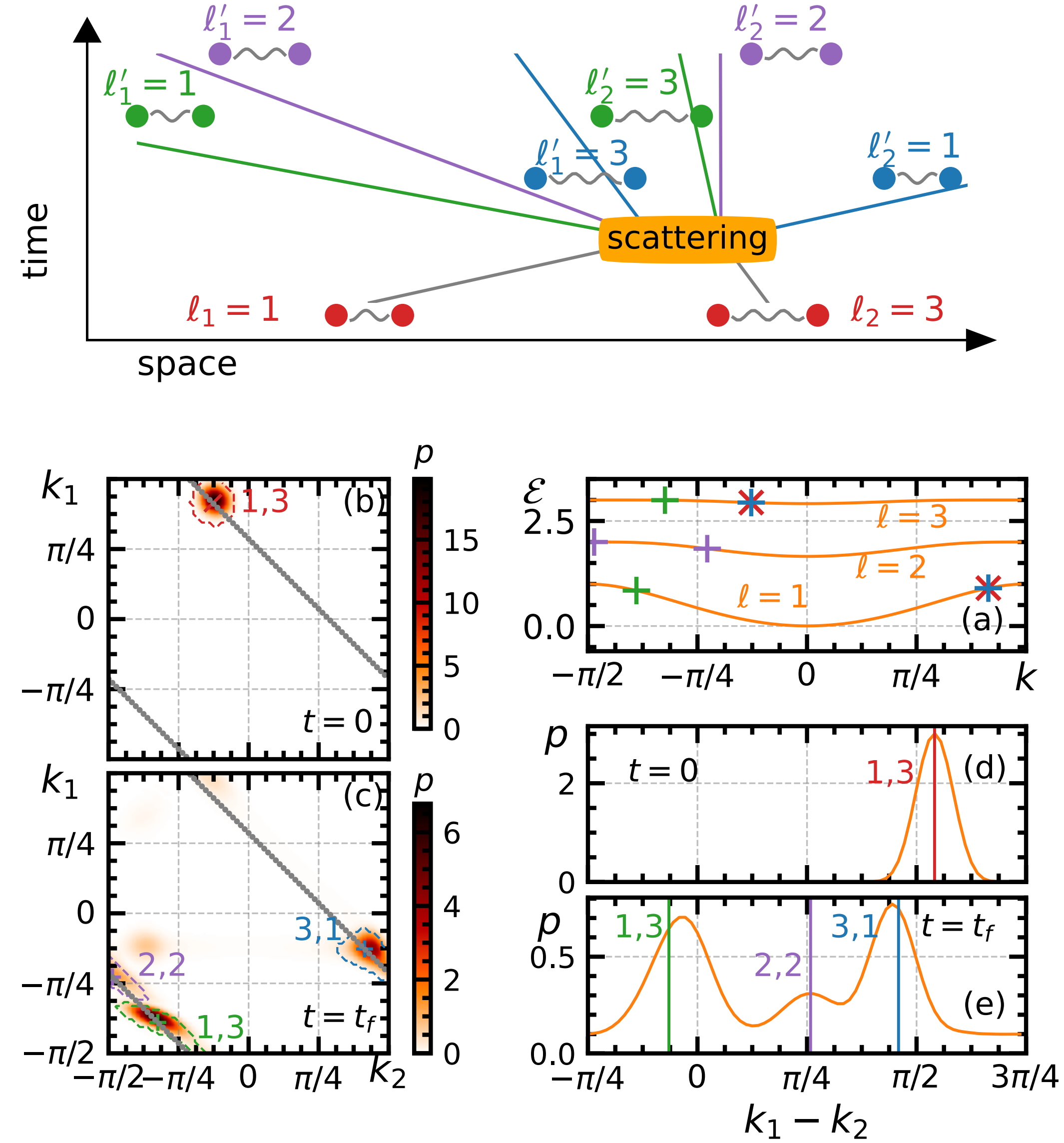
$q\bar{q}$ moving in medium

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

FIRST STEPS TOWARD SCATTERING IN SPIN SYSTEMS — NUMERICAL SIMULATIONS —



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

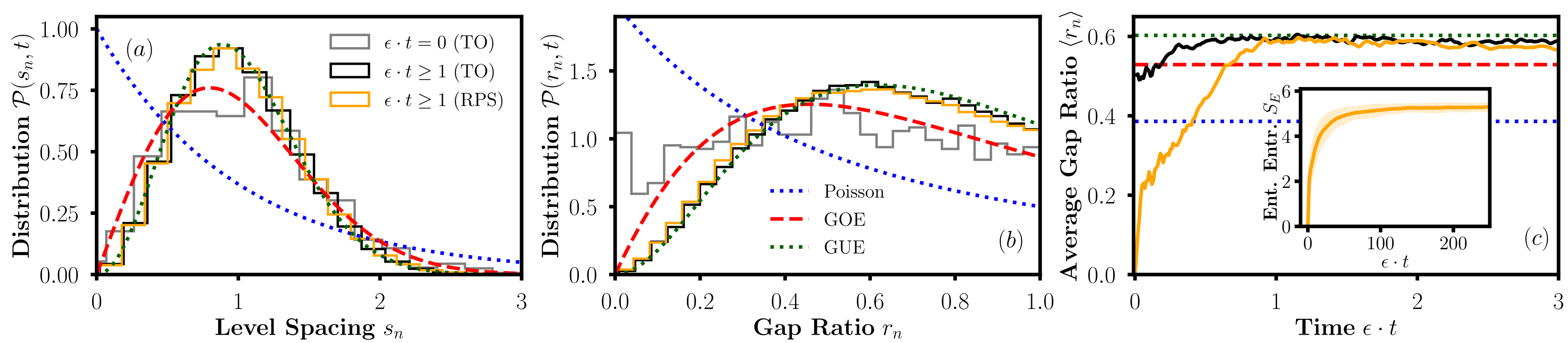


Surace, Lerose, New J. Phys. 23 (2021) 062001.

EMERGING UNDERSTANDING OF THERMALIZATION IN SIMPLE GAUGE THEORIES

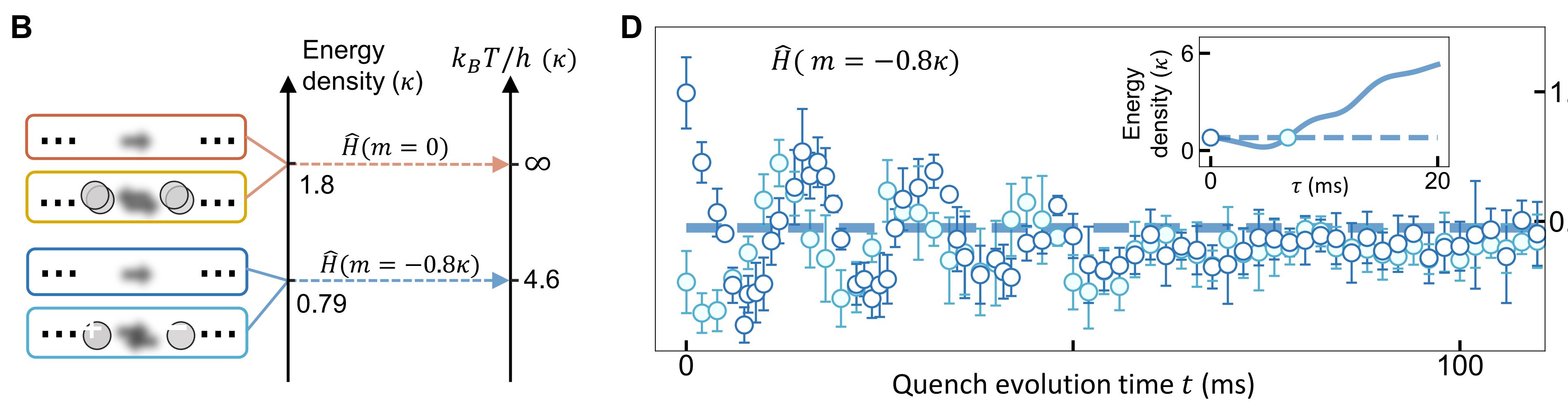
Numerical study of Z_2 LGT in 2+1 D

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

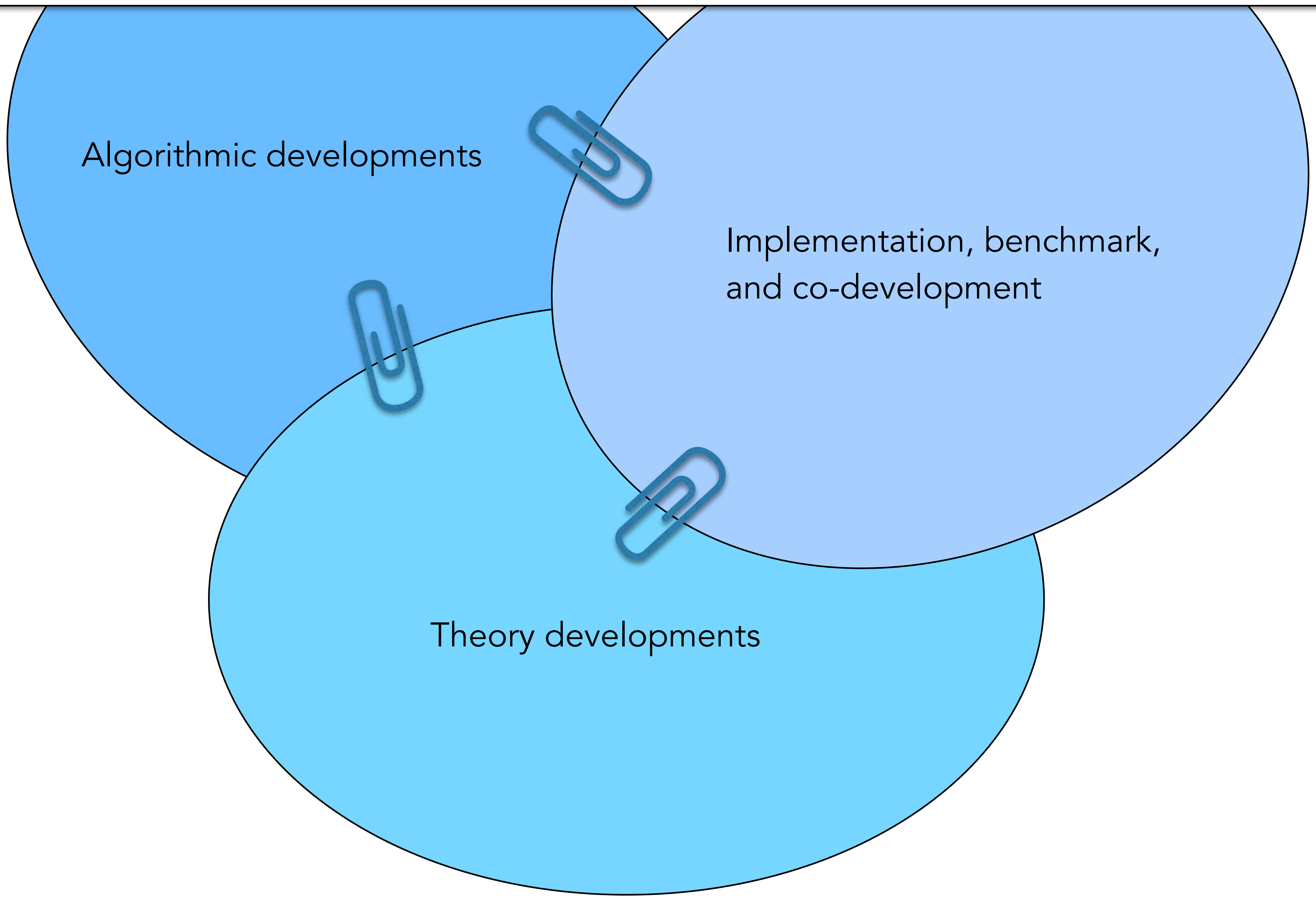


Quantum Link Model in a 70-site analog simulator

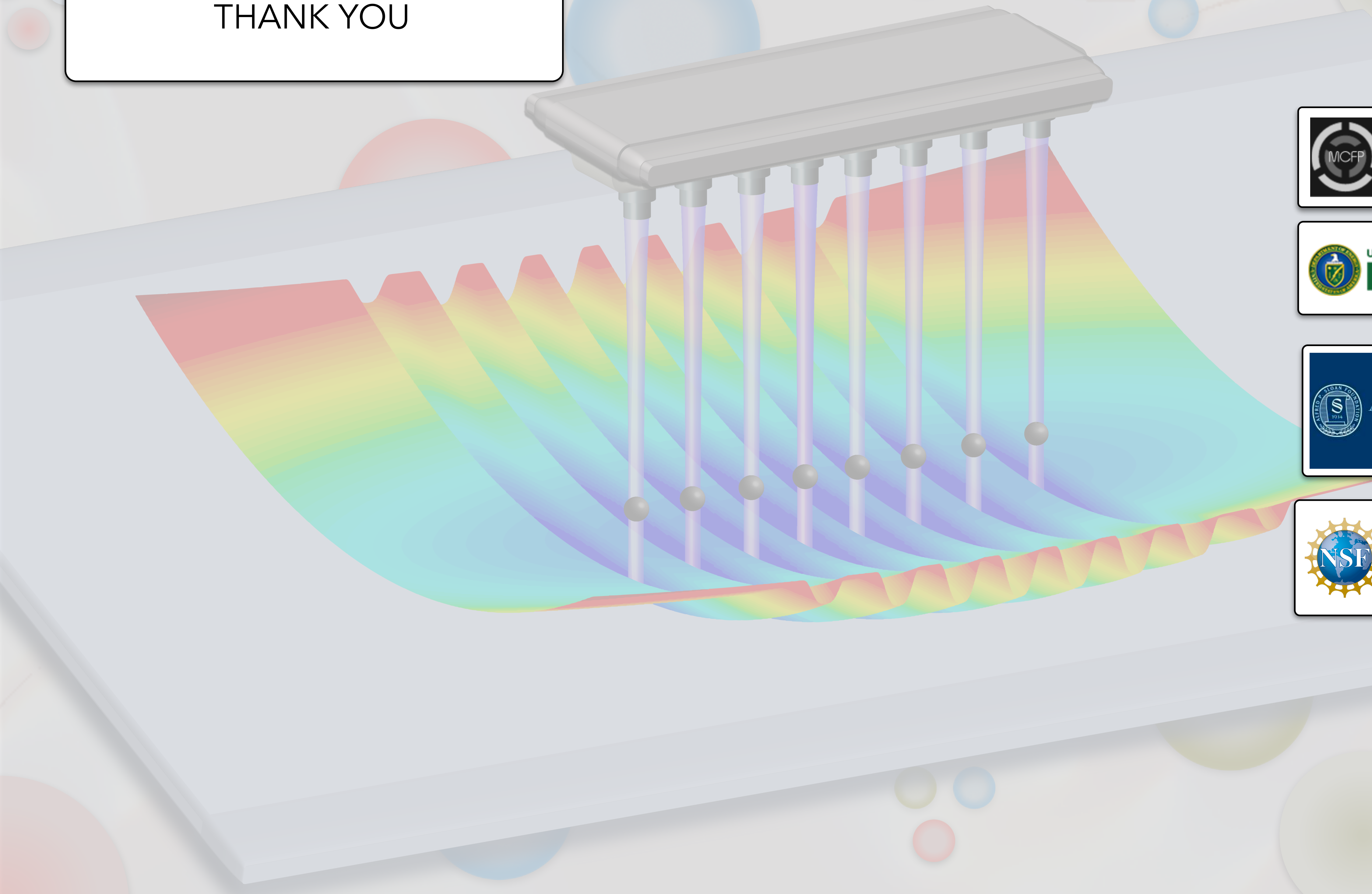
Zhou et al, *Science* 377 (2022) 6603.



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!



THANK YOU



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