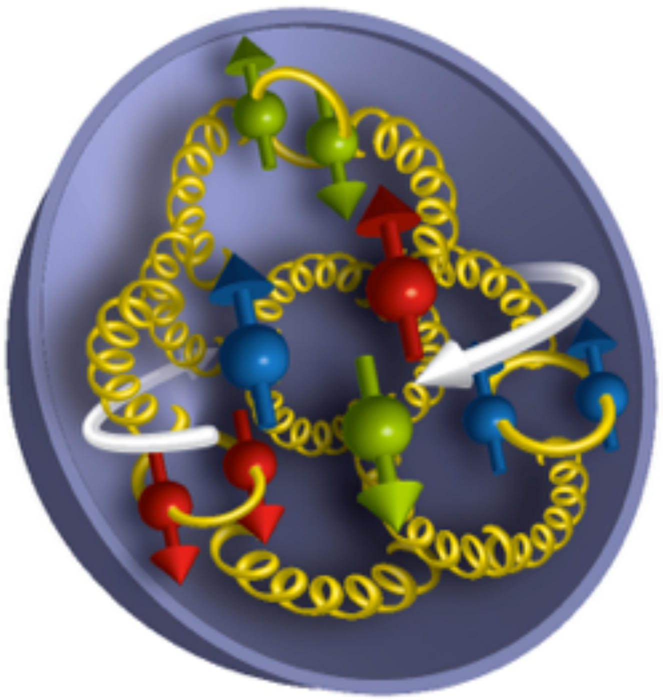
Quantum Computing Quantum Field Theories for Nuclear Physics

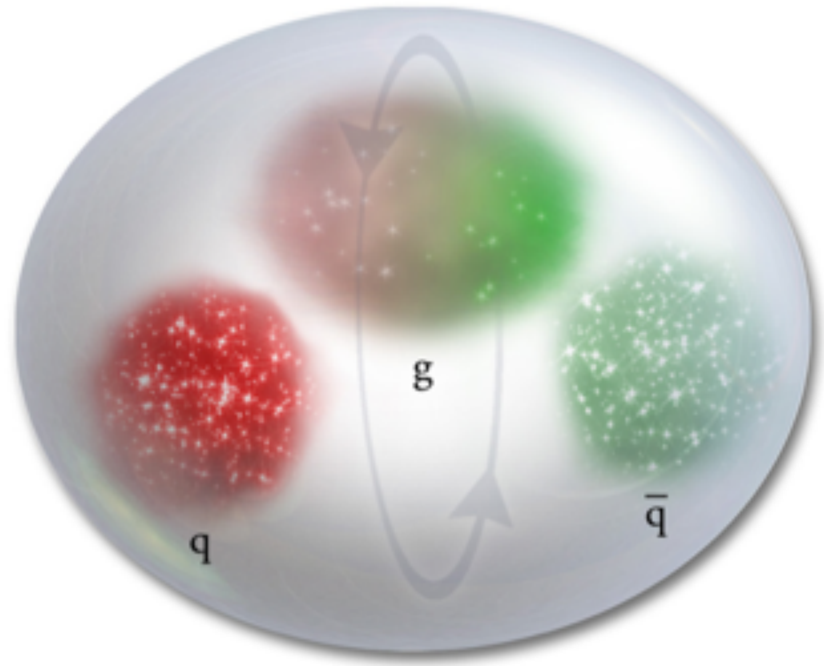
Martin J Savage

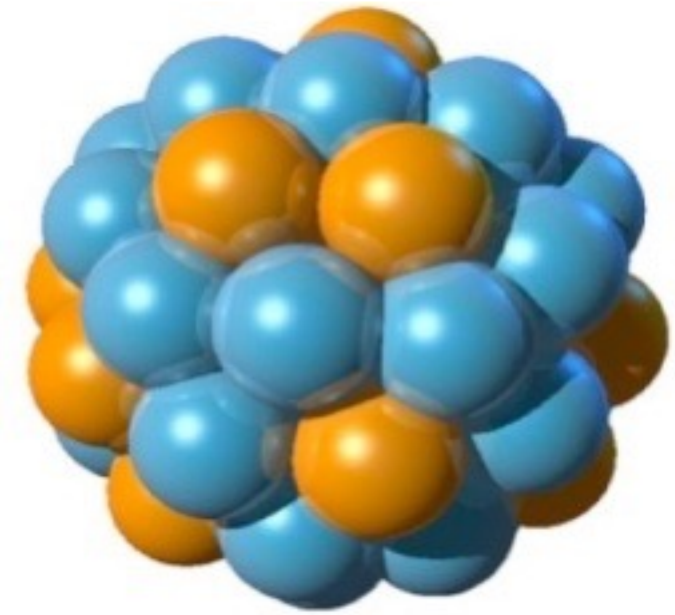
INT Workshop - Quantum Computing for Nuclear Physics
Seattle, November 14,15 , 2017

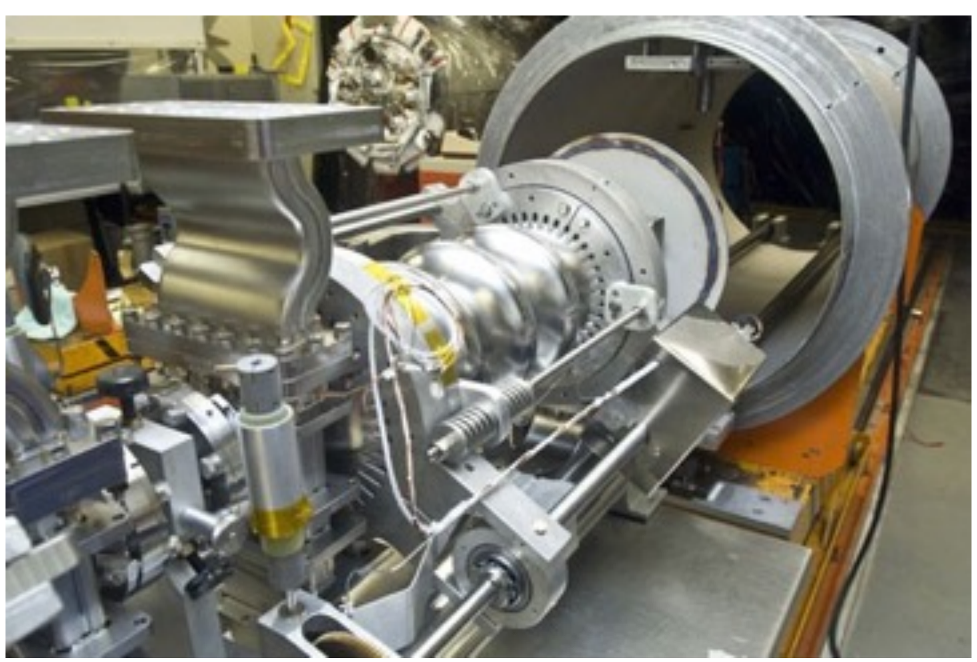
Institute for Nuclear Theory
University of Washington

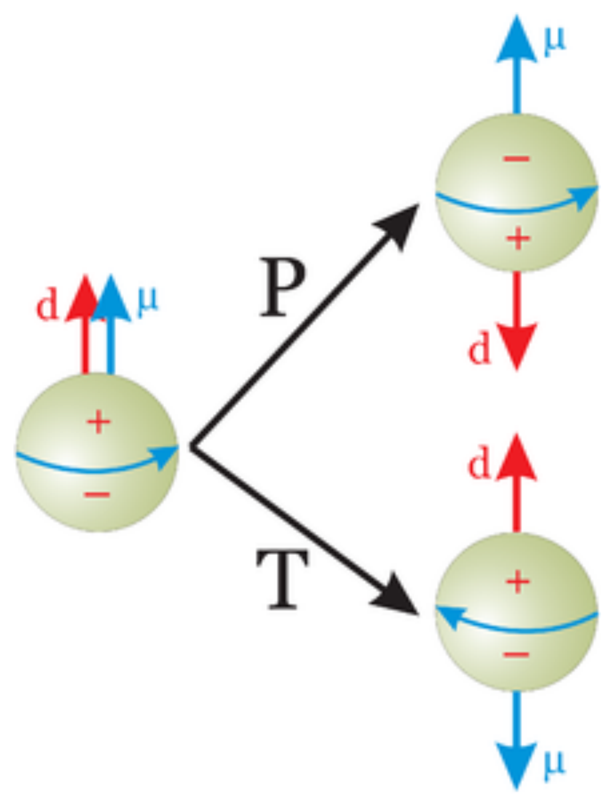
Hadrons and Nuclei

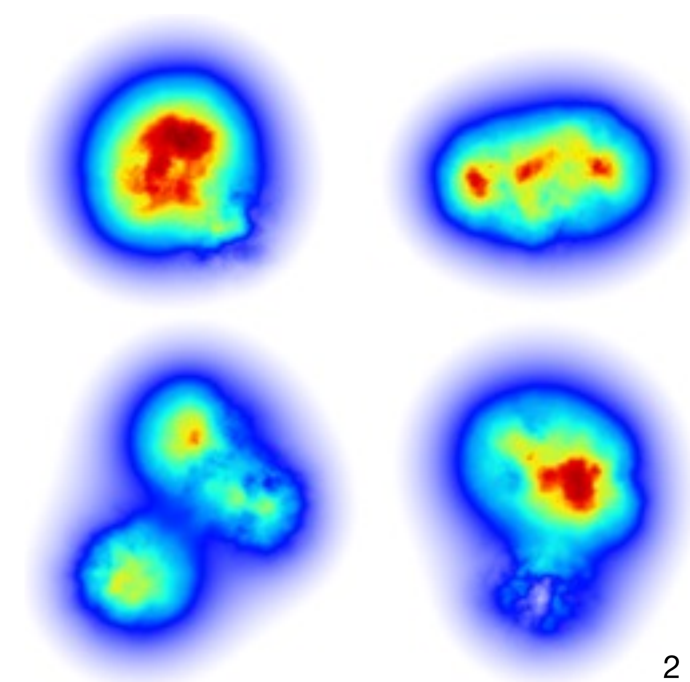




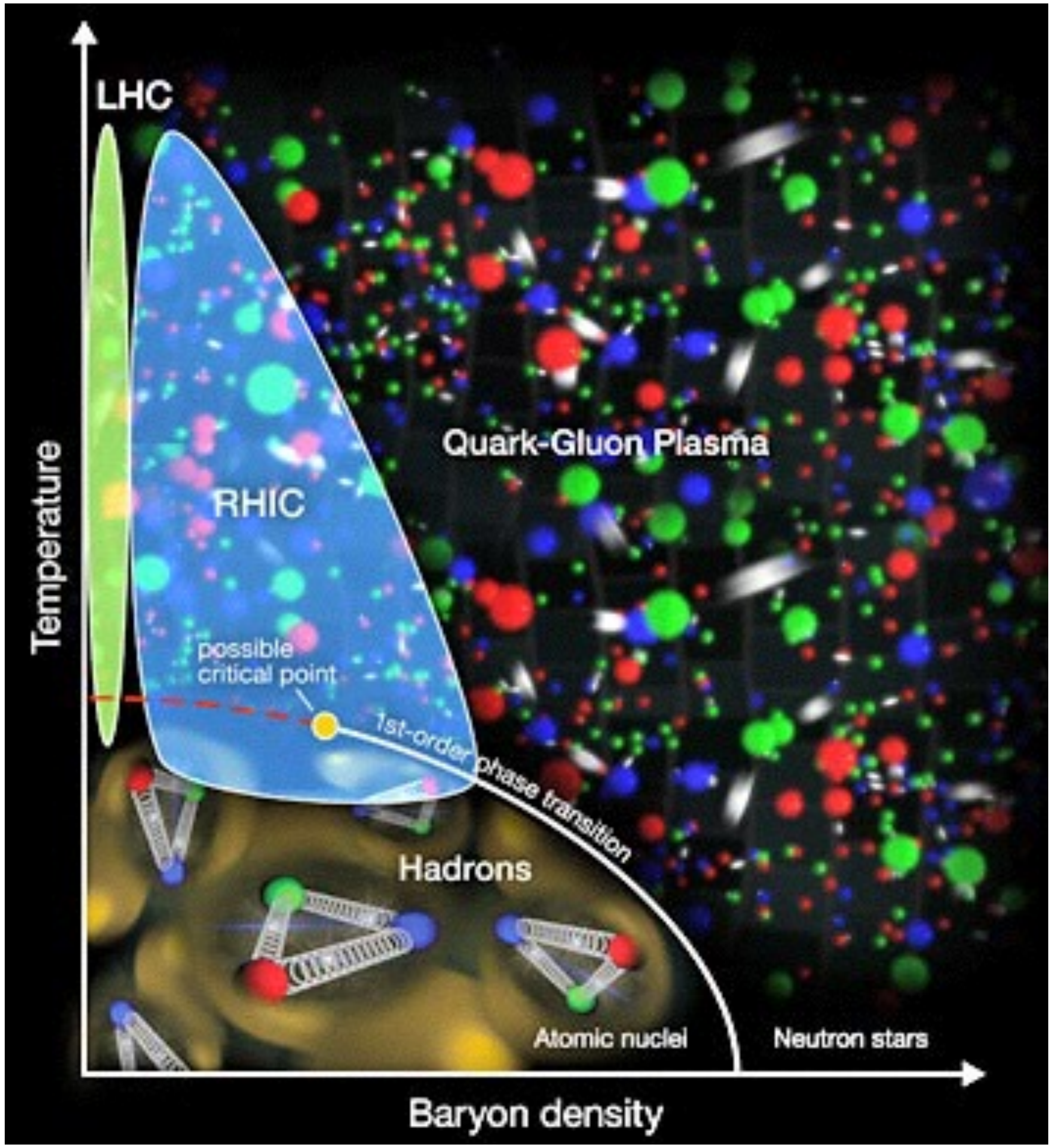


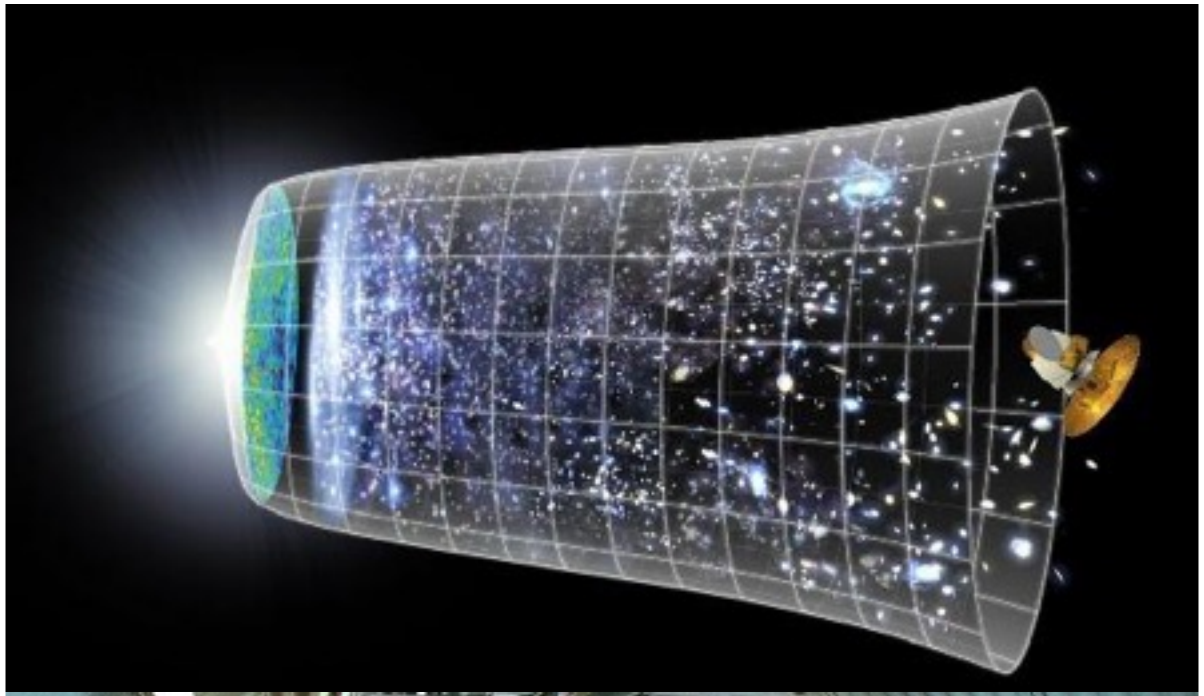


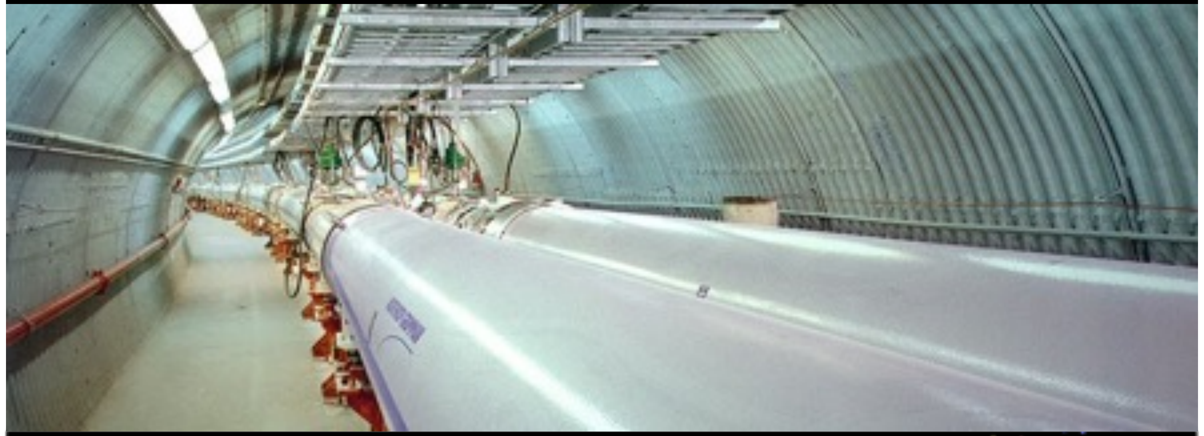


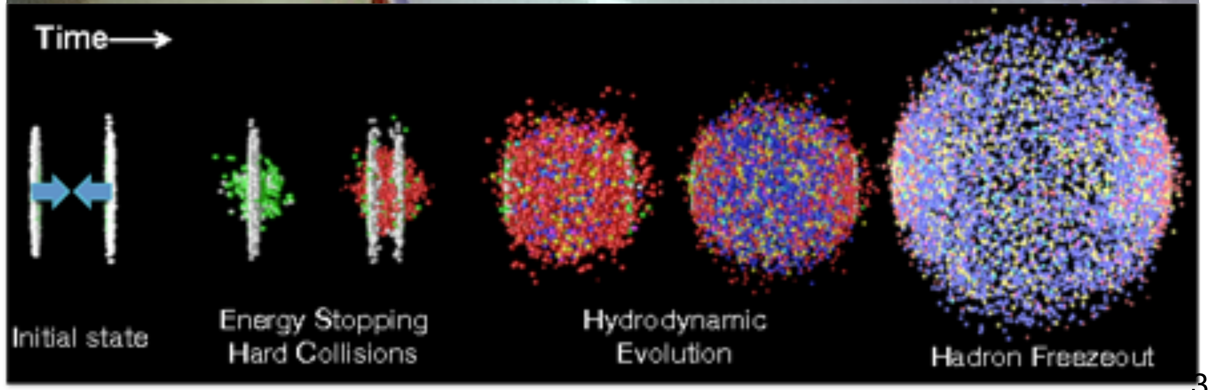


Hot and Dense Matter

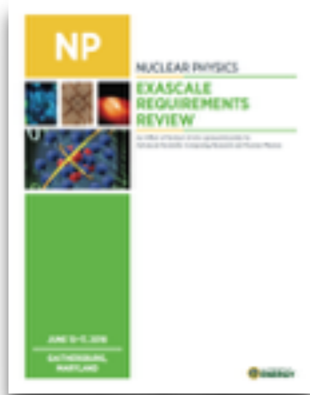






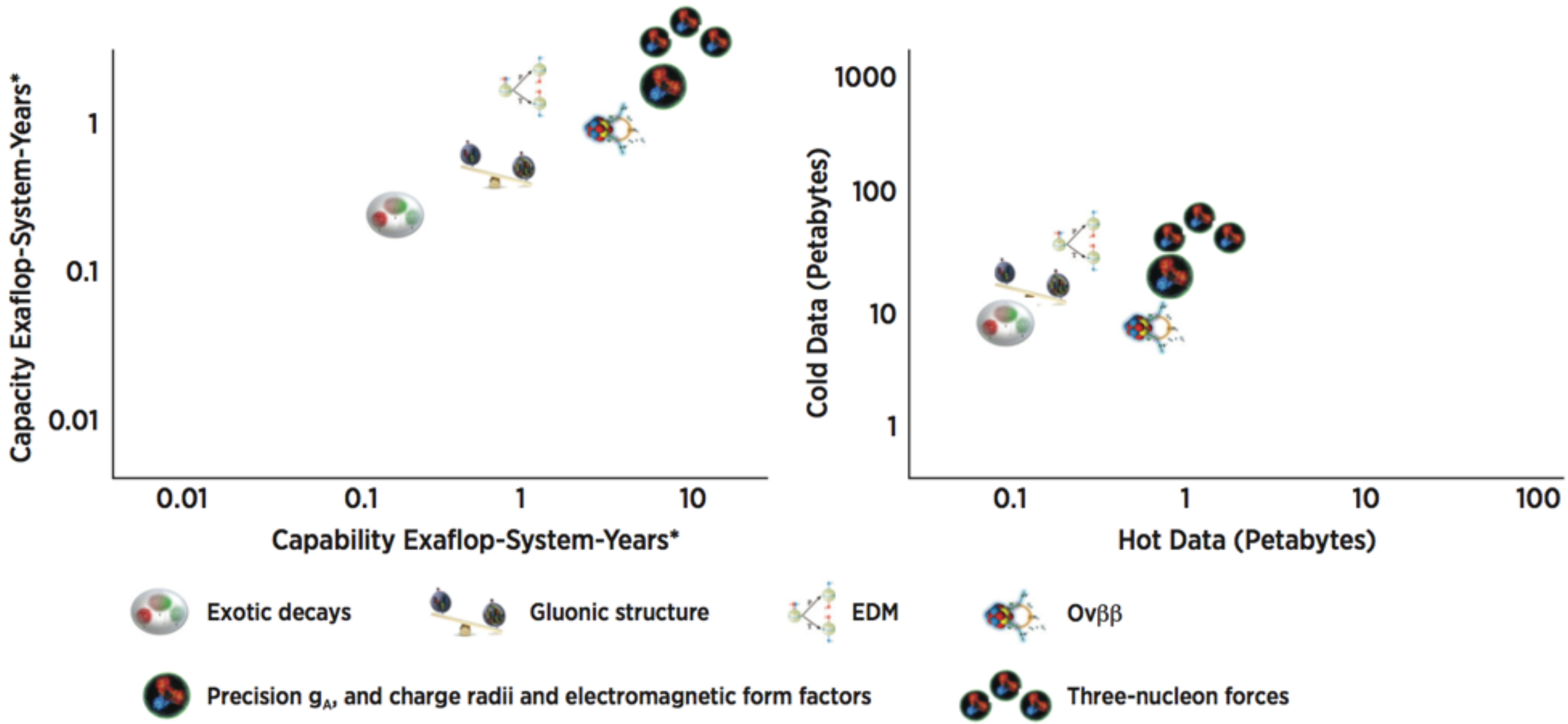


See talk by Peter Petrezcky tomorrow



Exascale Ecosystem for Nuclear Physics

CAPABILITY/CAPACITY RESOURCES VS. HOT/COLD DATA RESOURCES IN 2025
COLD QCD

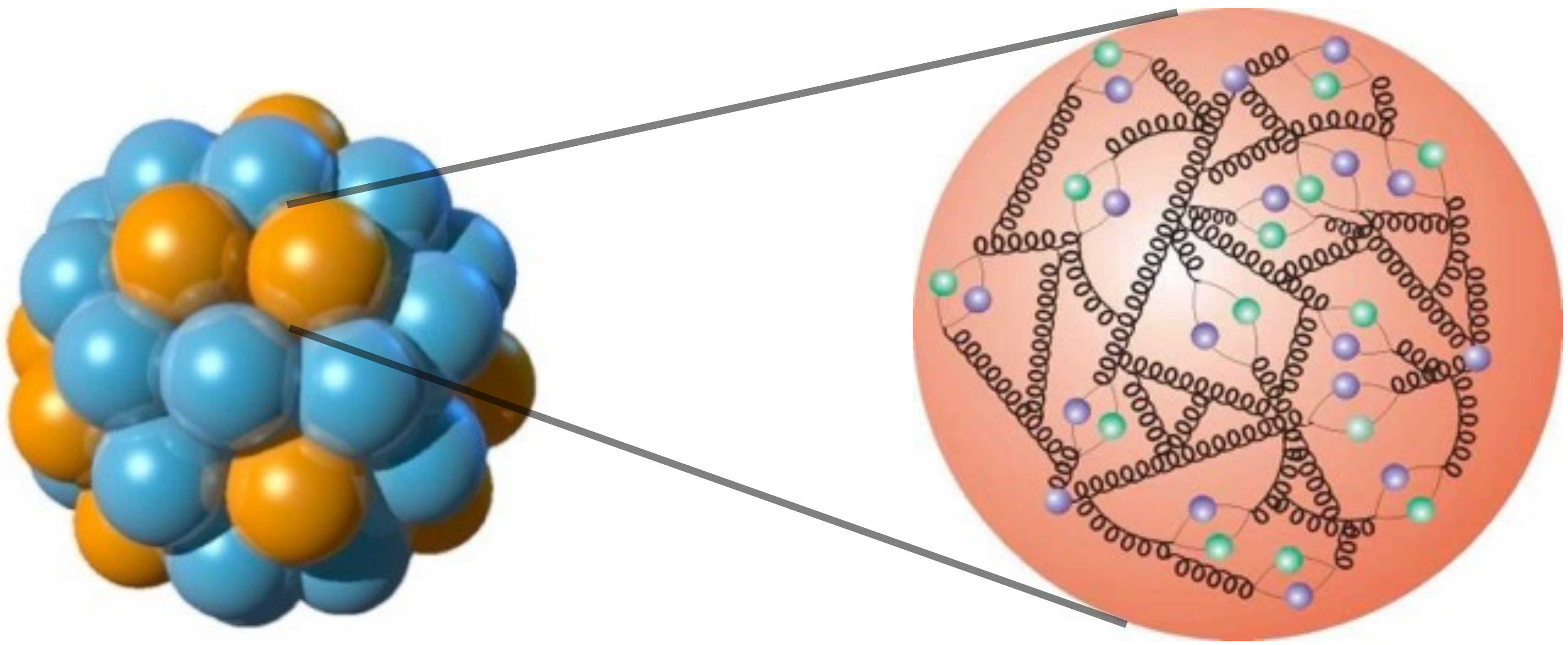


* Exaflop-system-year refers to the total amount of computation produced by an exascale computer in 1 year.

A single Exascale machine will be immediately oversubscribed by a large factor

Quantum Chromodynamics and NP

Nucleus | Proton



Protons and Neutrons | Quarks and Gluons

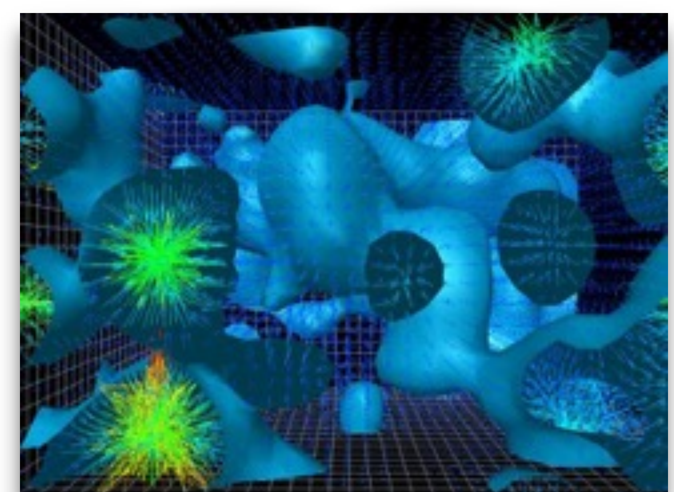
Goal #0 : calculate the mass of the proton

Quantum Chromodynamics
Path Integrals and Lattice QCD

Minkowski Space - probability amplitudes of unit norm

$$Z \;\propto \int \mathcal{D}A^a_\mu \mathcal{D}\overline{q}_i \mathcal{D}q_i \; e^{\frac{i}{\hbar}\int d^4x \;\mathcal{L}+\mathcal{L}_{g.f.}+\mathcal{L}_{\rm ghosts}}$$

$$\mathcal{L} = \sum_{i=u,d,s,c,b,t} \overline{q}_i \left[\, i\not{D} - m_i \,\right] q_i \; - \; \frac{1}{4} \sum_{a=1,...,8} G^a_{\mu\nu} G^{\mu\nu,a}$$



Euclidean Space - probability distribution

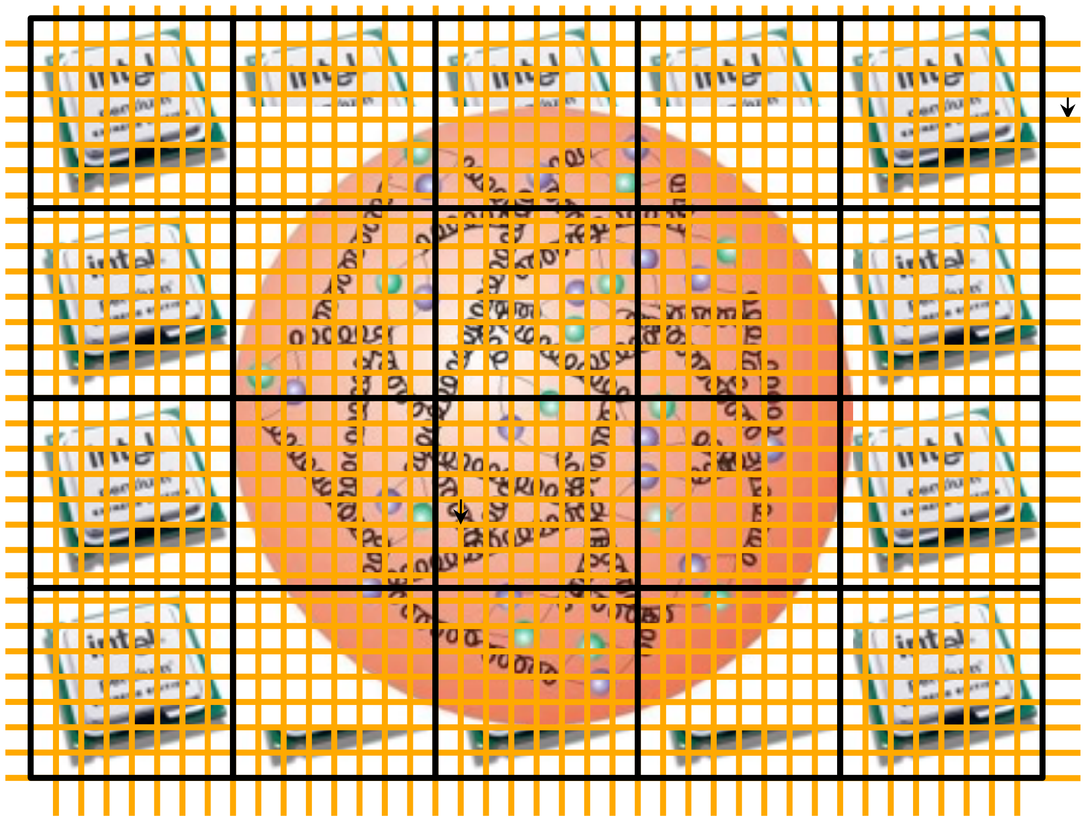
$$\langle \hat{\theta} \rangle \sim \int \mathcal{D}\mathcal{U}_\mu \; \hat{\theta}[\mathcal{U}_\mu] \; \det[\kappa[\mathcal{U}_\mu]] \; e^{-S_{YM}}$$

$$\rightarrow \frac{1}{N} \sum_{\rm gluon\;\; cfgs}^{N} \hat{\theta}\,[\mathcal{U}_\mu]$$

Gauge fields sampled

Fermion integrals can be performed analytically

Lattice Quantum Chromodynamics - Discretized Euclidean Spacetime

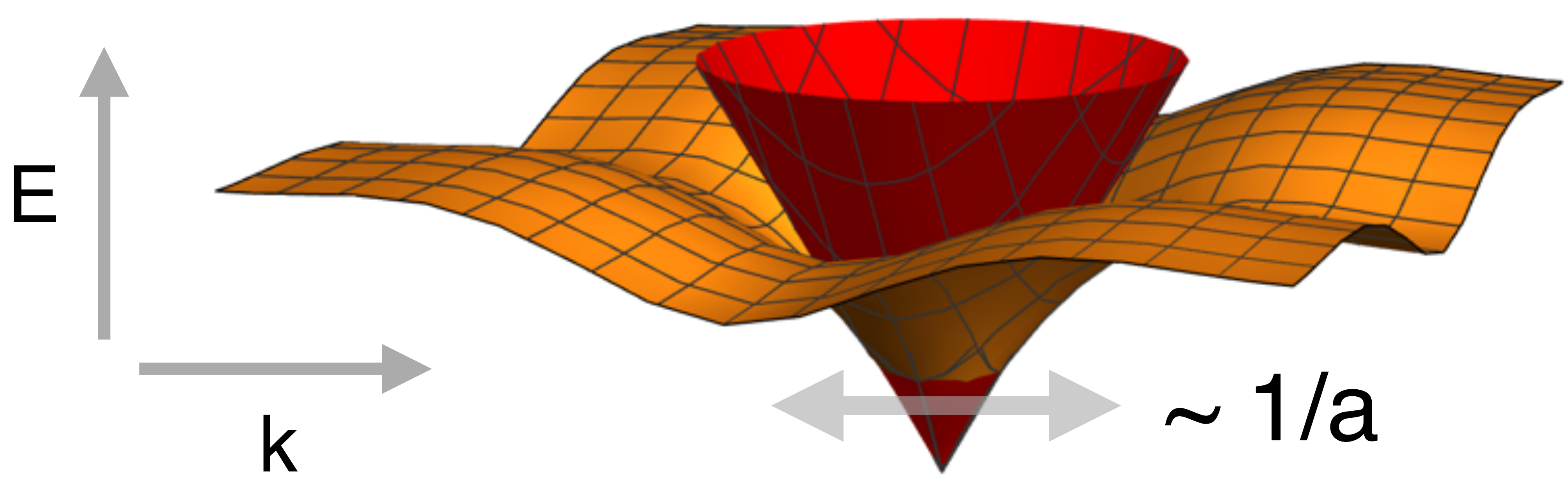


Lattice Spacing : $a << 1/\Lambda\chi$ (Nearly Continuum)

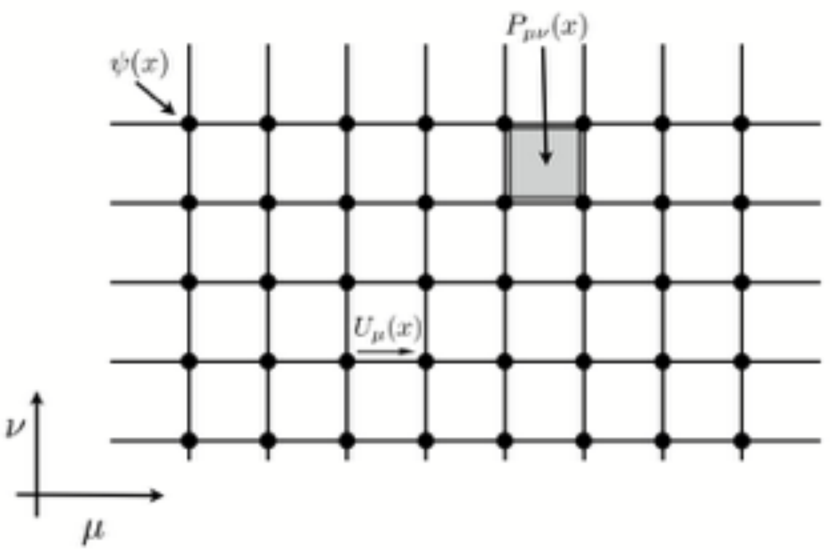
Lattice Volume : $m_\pi L >> 2\pi$ (Nearly Infinite Volume)

Extrapolation to $a = 0$ and $L = \infty$

Systematically remove non-QCD parts of calculation through effective field theories



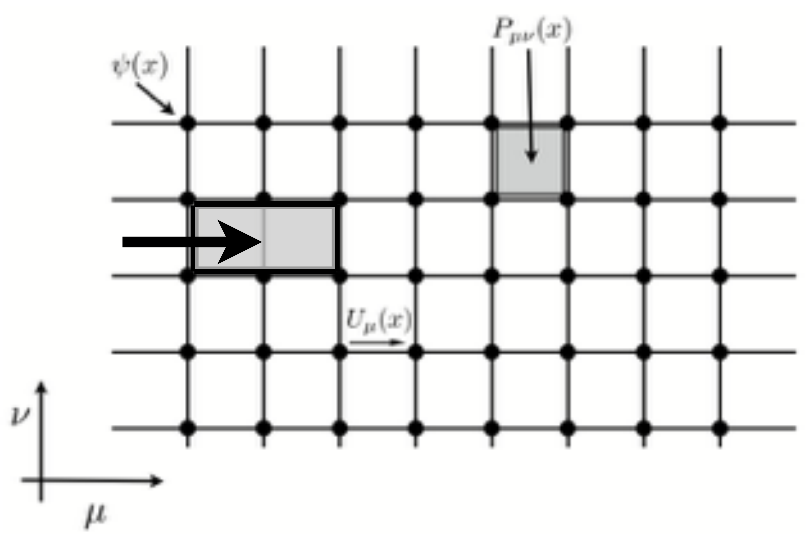
Lattice QCD
The Discretized Action



$$U_\mu(x) = \exp\left(i \int_x^{x+\hat{\mu}} dx' A_\mu(x')\right)$$

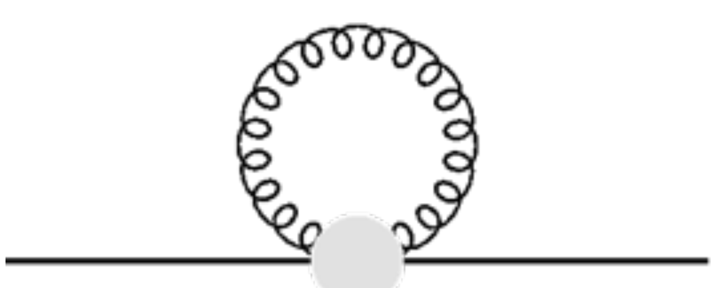
$$U_\mu(x) \rightarrow U'_\mu(x) = \Omega(x) U_\mu(x) \Omega^{-1}(x+\hat{\mu})$$

$$P_{\mu\nu} = U_\mu(x) U_\nu(x+\hat{\mu}) U^\dagger_\mu(x+\hat{\nu}) U^\dagger_\nu(x)$$



$$S_{\text{classical}} \equiv -\beta \sum_{x,\mu>\nu} \left\{ \frac{5P_{\mu\nu}}{3} - \frac{R_{\mu\nu}+R_{\nu\mu}}{12} \right\} + \text{const}$$

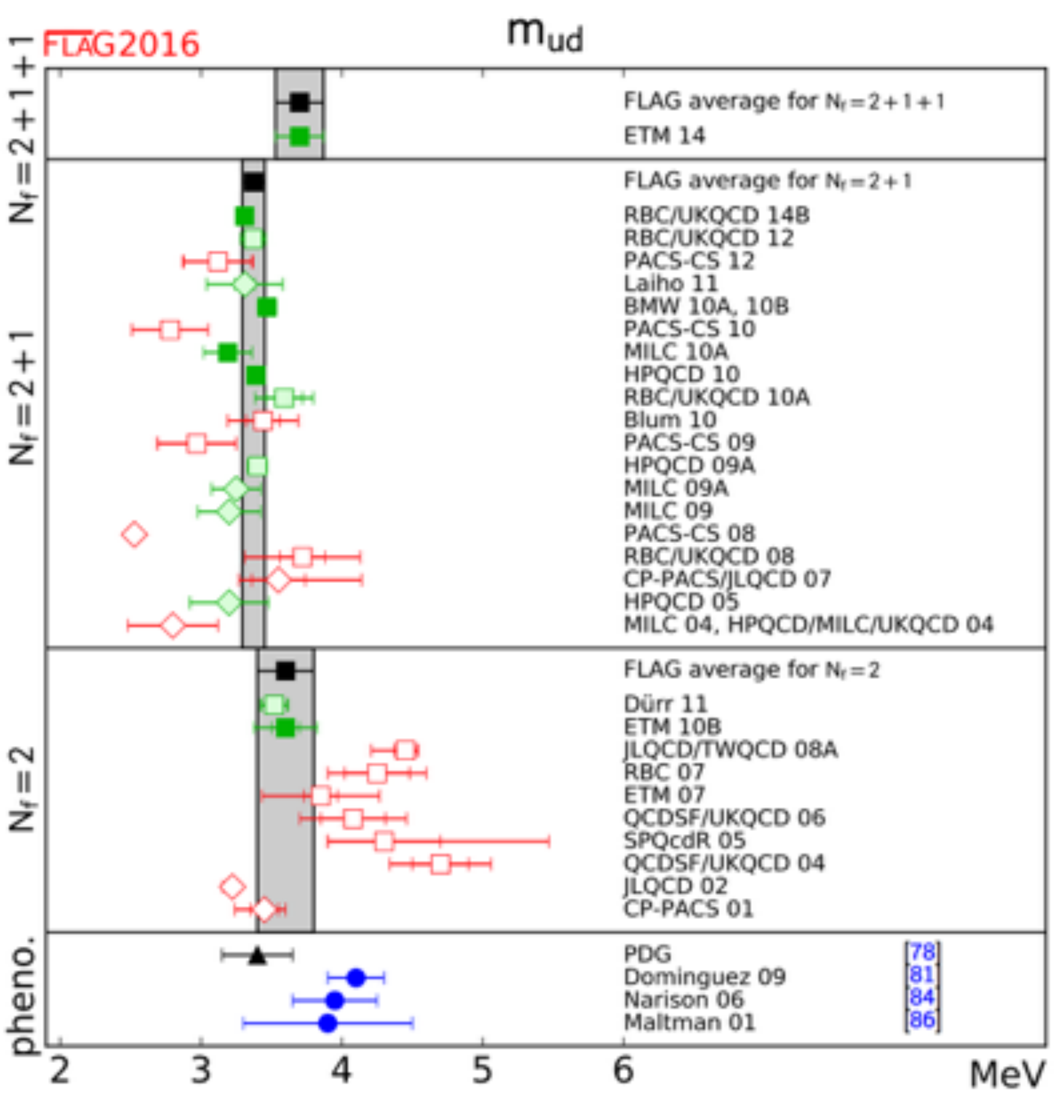
$$= \int d^4x \sum_{\mu,\nu} \tfrac{1}{2} \operatorname{Tr} F^2_{\mu\nu} + \mathcal{O}(a^4).$$

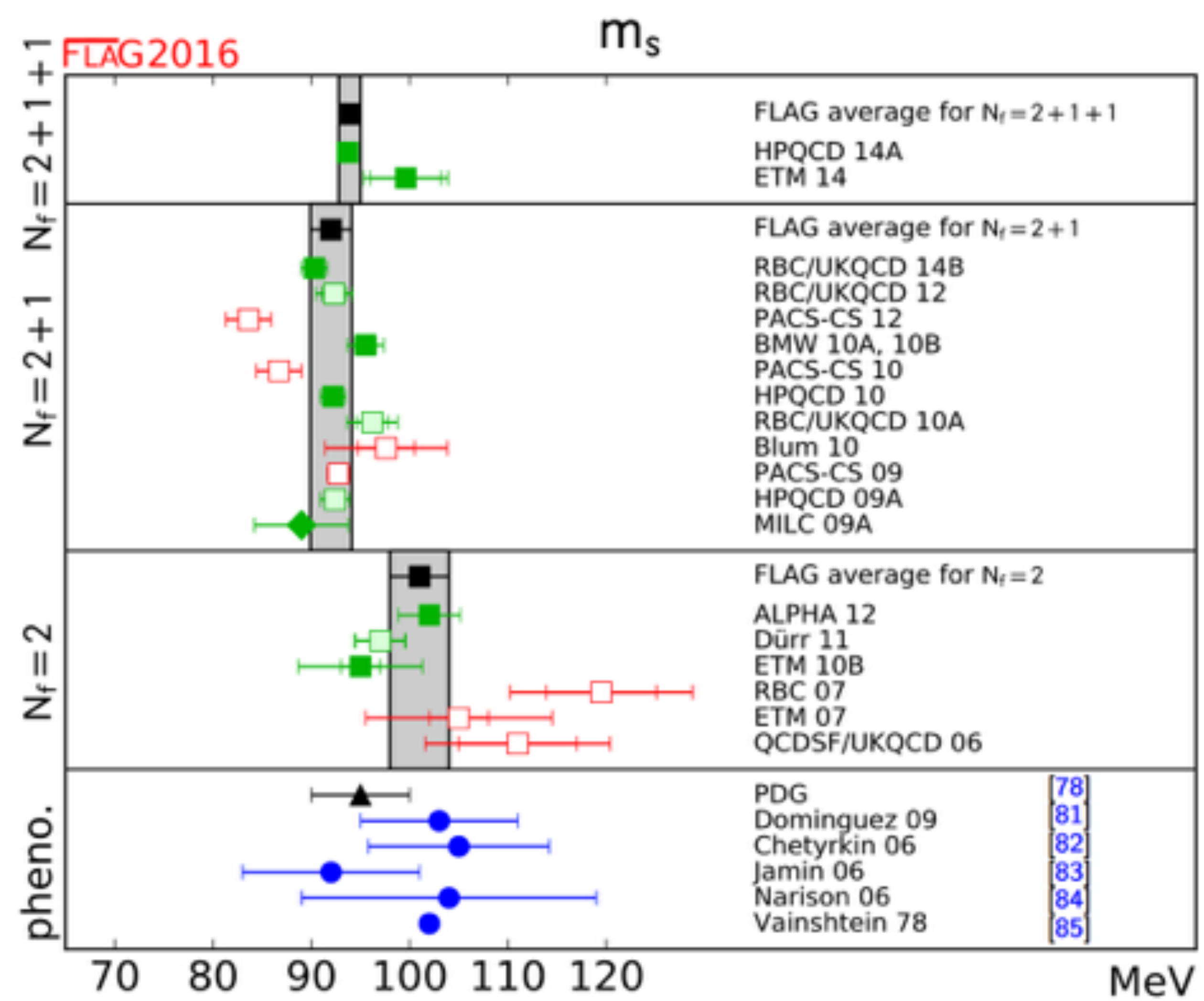


$$S = -\beta \sum_{x,\mu>\nu} \left\{ \frac{5}{3}\frac{P_{\mu\nu}}{u_0^4} - \frac{R_{\mu\nu}+R_{\nu\mu}}{12\,u_0^6} \right\}$$

Quantum gauge action tadpole improved

Lattice QCD
The Quark Masses





N_f	m_u	m_d	m_u/m_d
2+1	2.16(9)(7)	4.68(14)(7)	0.46(2)(2)
2	2.40(23)	4.80(23)	0.50(4)

$$\overline{\mathrm{MS}}\ ,\ \mu = 2\ \mathrm{GeV}$$

Lattice QCD
Sketch of Methodology

Start with a selection of quark+gluon sources and sinks ``designed'' to have good overlap onto the low-lying hadronic/nuclear states in the volume.

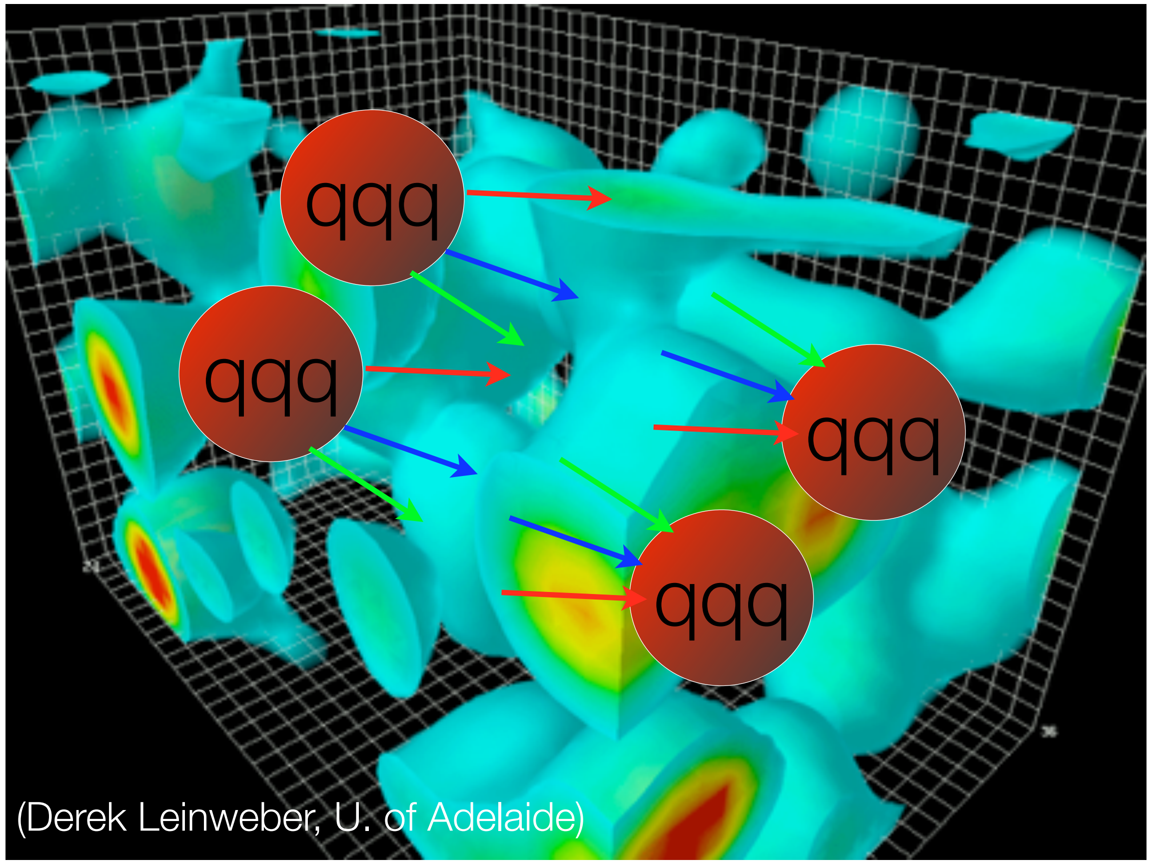
Iteratively (manually) refine to produce ``best estimates'' of QCD states.

Form correlation functions between all combinations

Diagonalize to find the energy eigenvalues and eigenstates (Variational or other)

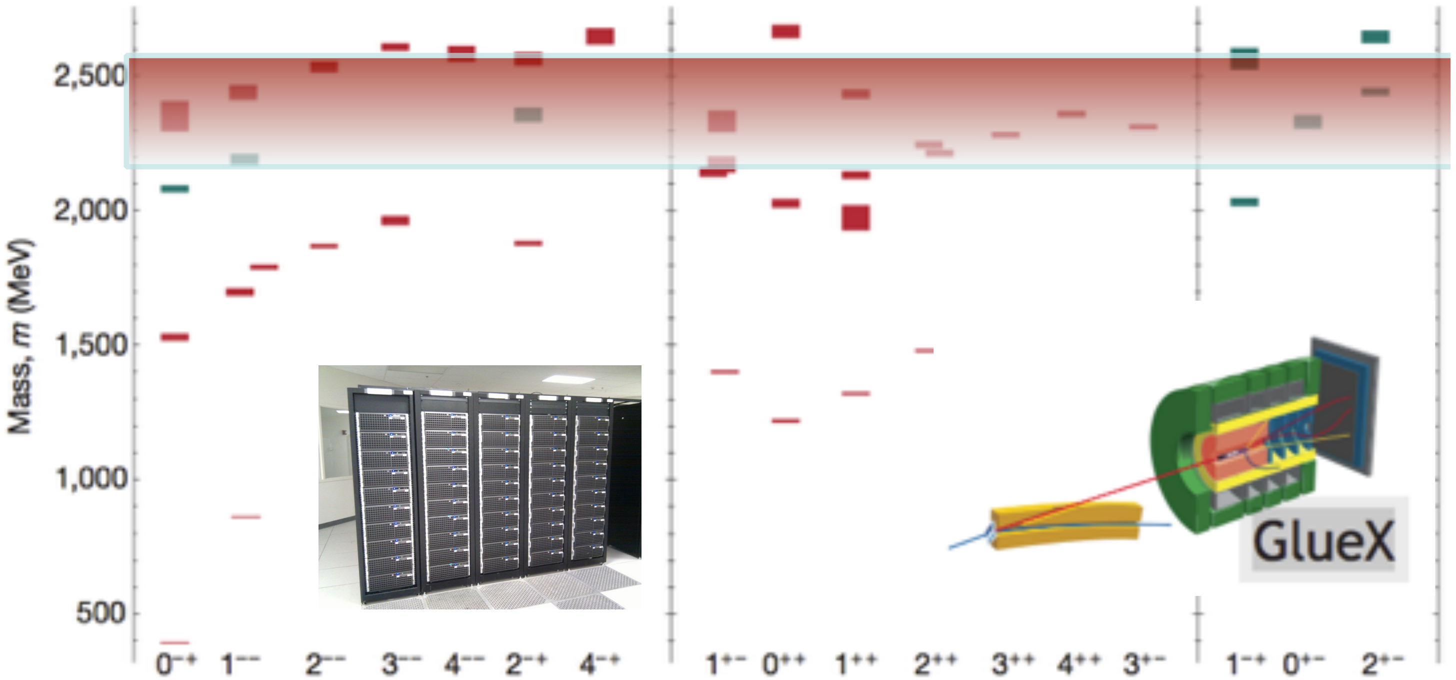
Post-analyze accordingly
- Luscher's Methods for S-matrix elements,…

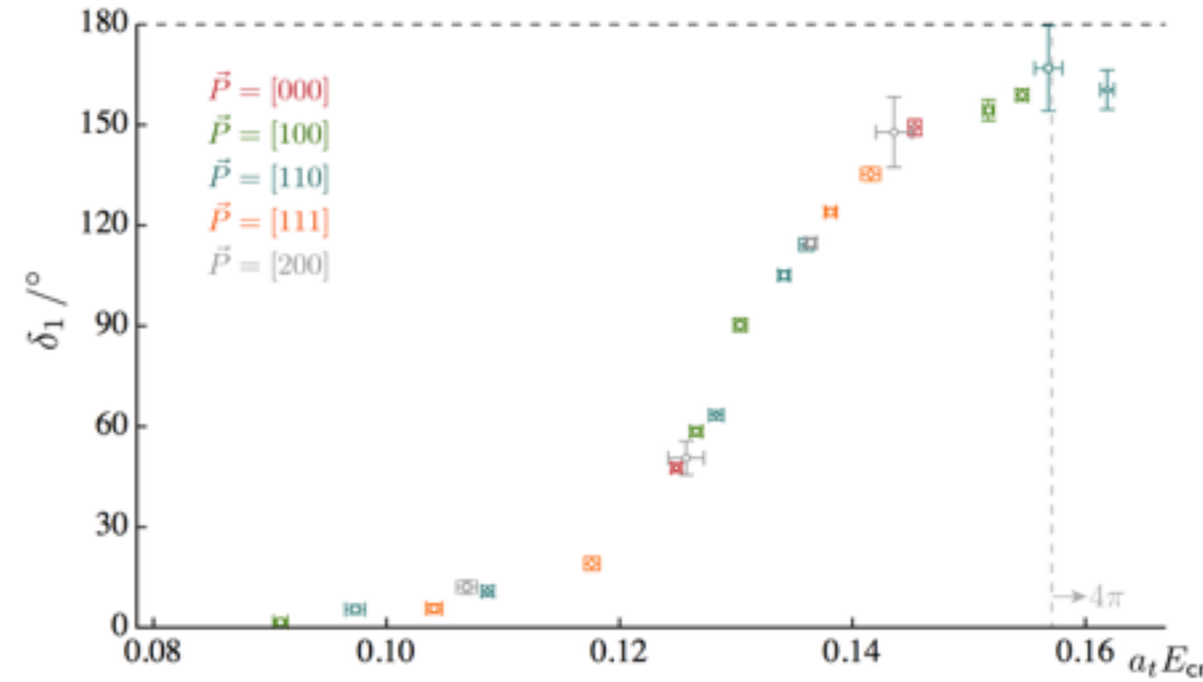
Don't try to do everything - way to complex
- focus on low-lying states and processes



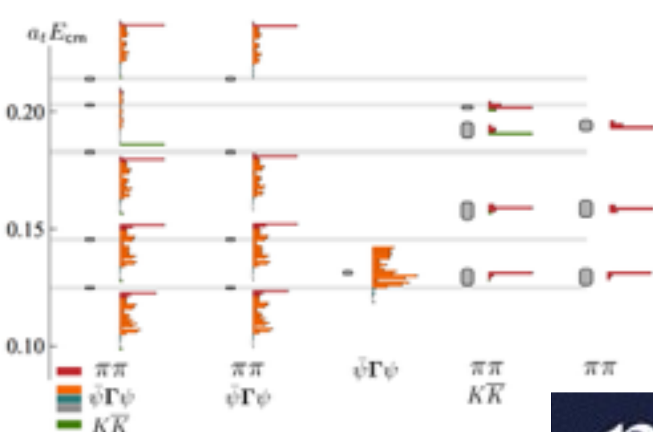
(Derek Leinweber, U. of Adelaide)

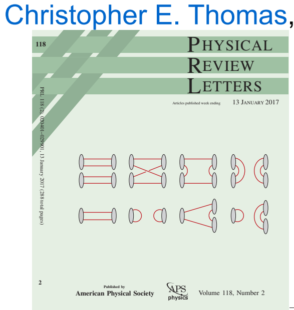
Lattice QCD
Spectroscopy and GlueX



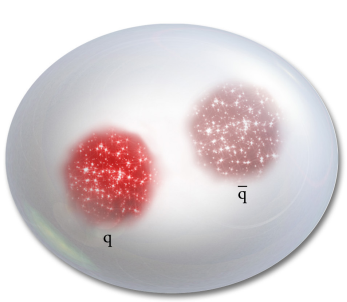


David J. Wilson, Raul A. Briceno, Jozef J. Dudek, Robert G. Edwards, Christopher E. Thomas, Phys.Rev. D92 (2015) no.9, 094502

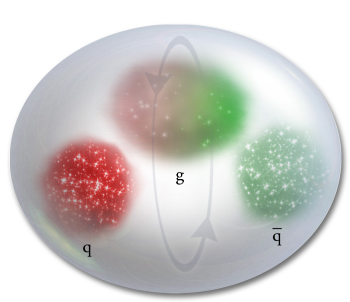




Pattern of states suggest gluonic excitations



Conventional Meson



Hybrid Meson

NATURE | REVIEW

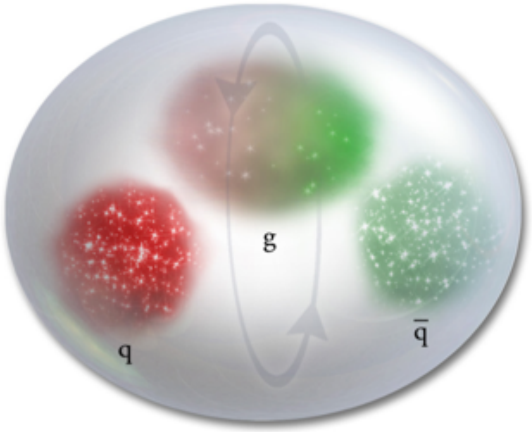
Searching for the rules that govern hadron construction

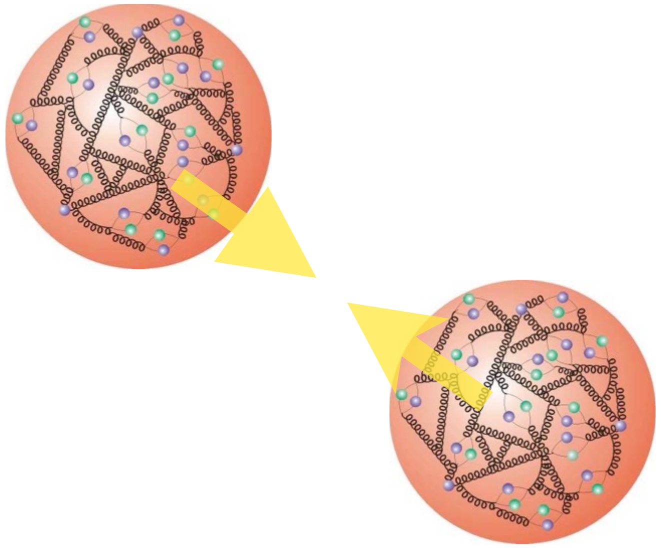
Matthew R. Shepherd, Jozef J. Dudek & Ryan E. Mitchell

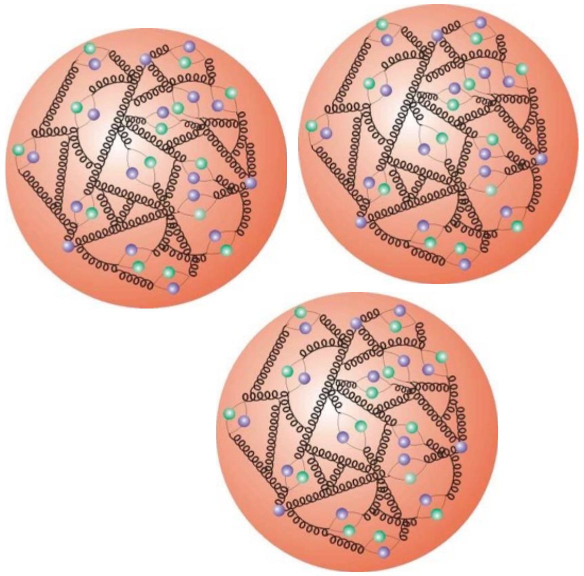
Nature **534**, 487–493 (23 June 2016) | doi:10.1038/nature18011

Systems to Explore
Quantum Computing Potential

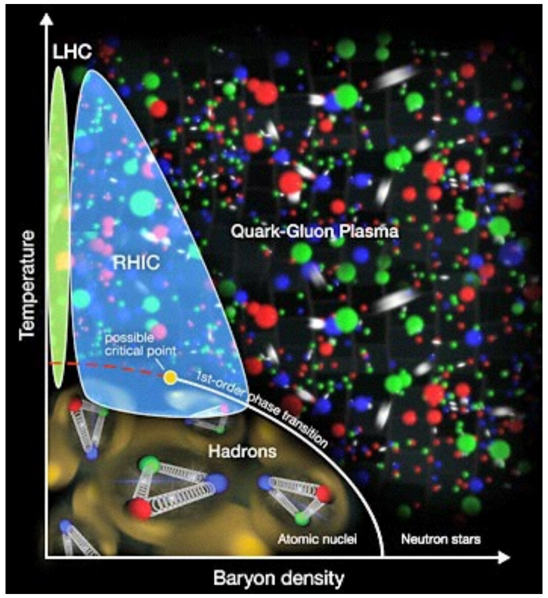
S-matrix elements, equilibrium properties, definite quantum numbers, e.g., 2 neutrons and 1 proton

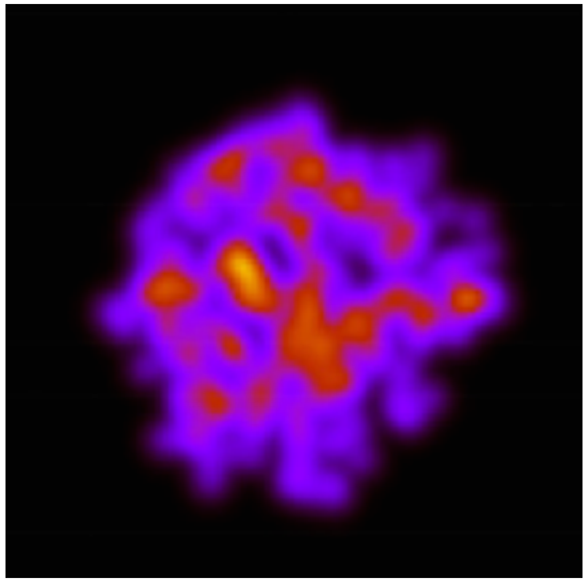


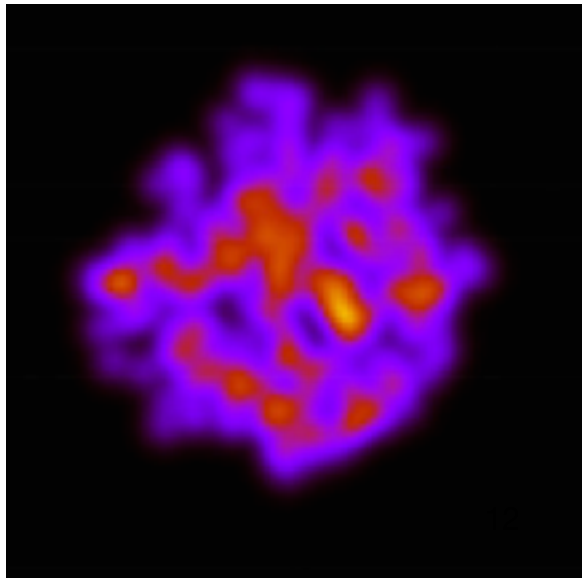




Time evolution of system with baryon number, isospin, electric charge, strangeness, …..
Currents, viscosity, non-equilibrium dynamics - real-time evolution



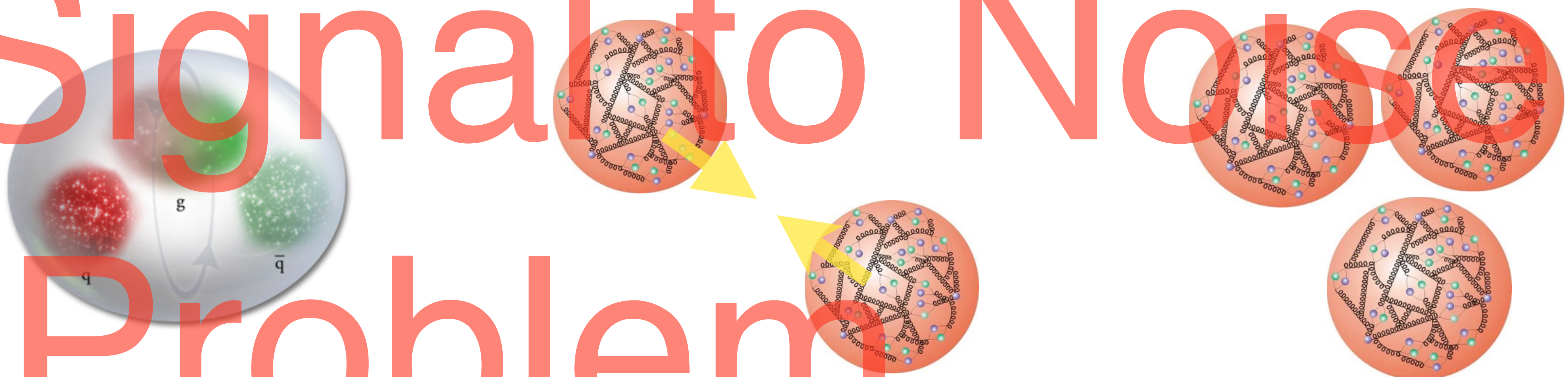




Systems to Explore Quantum Computing Potential

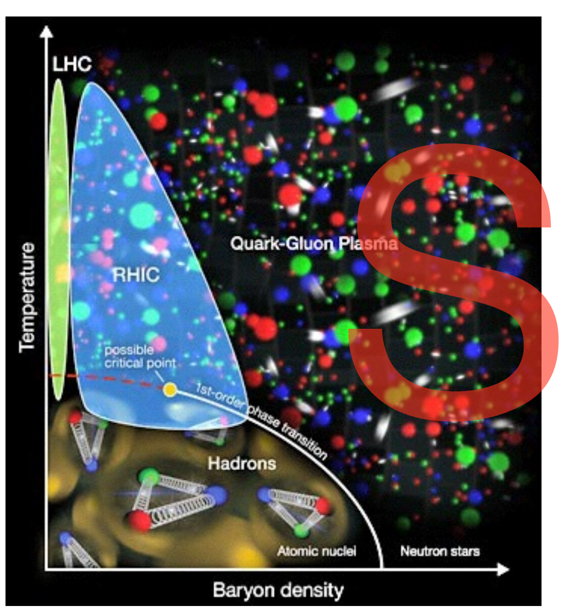
S-matrix elements, equilibrium properties, definite quantum numbers, i.e. 2 neutrons and 1 proton

Signal to Noise Problem

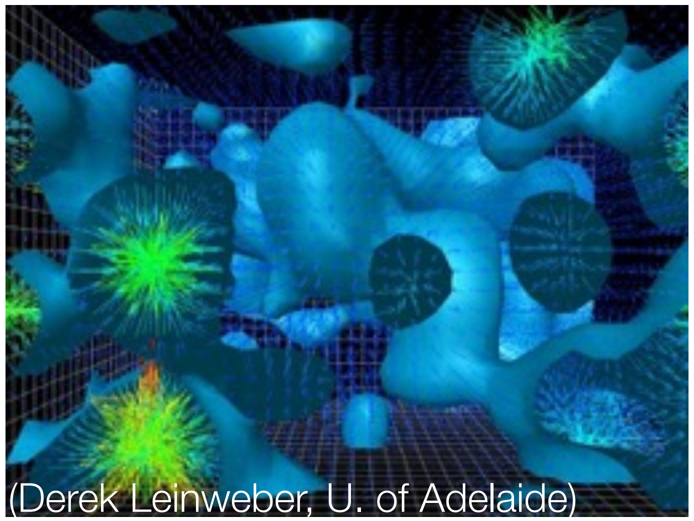


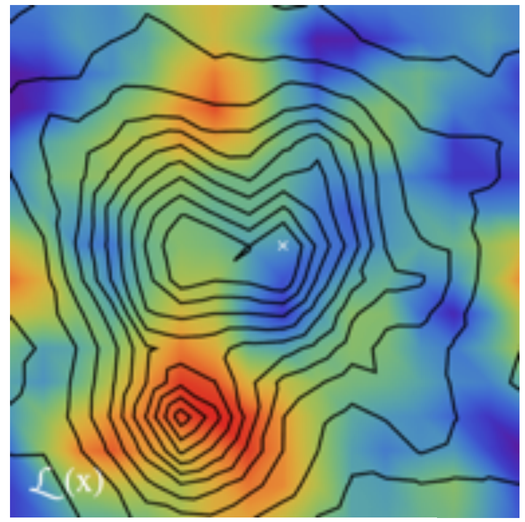
Time evolution of system with baryon number, isospin, electric charge, strangeness, …..
Currents, viscosity, non-equilibrium dynamics - real-time evolution

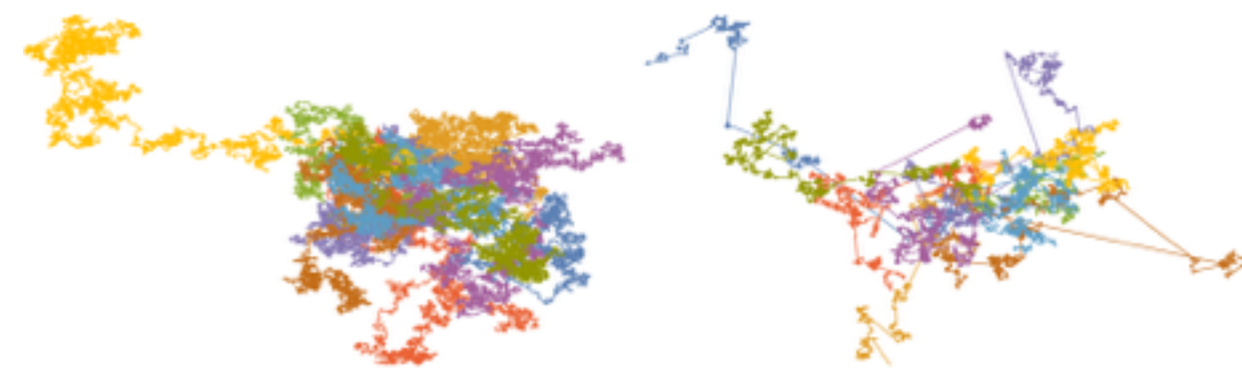
Sign Problem



Systems to Explore Quantum Computing Potential One Baryon and More

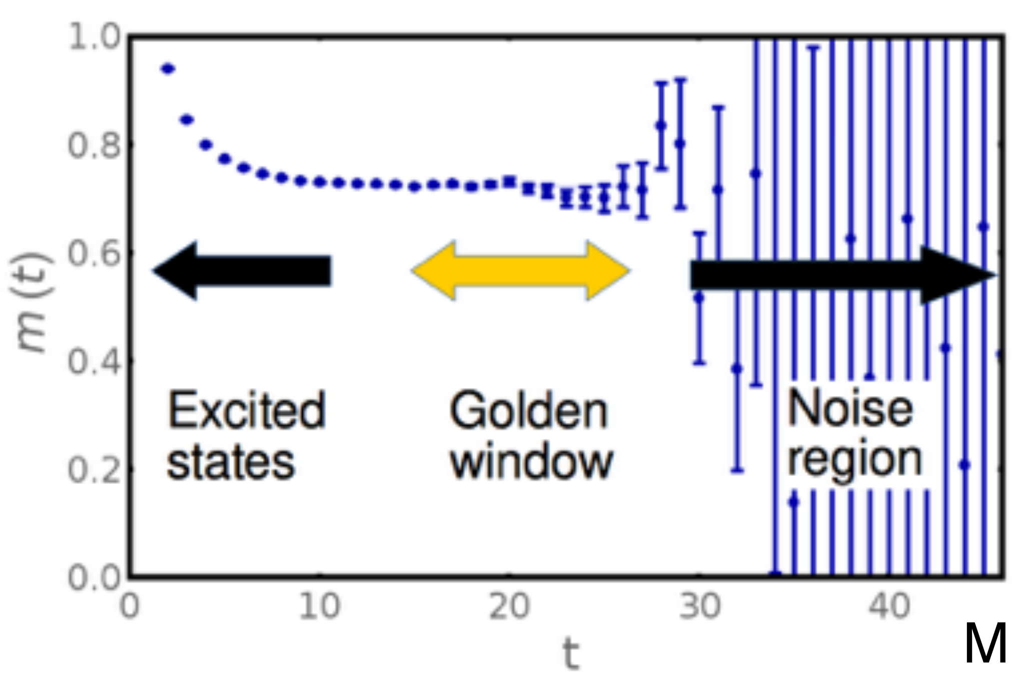


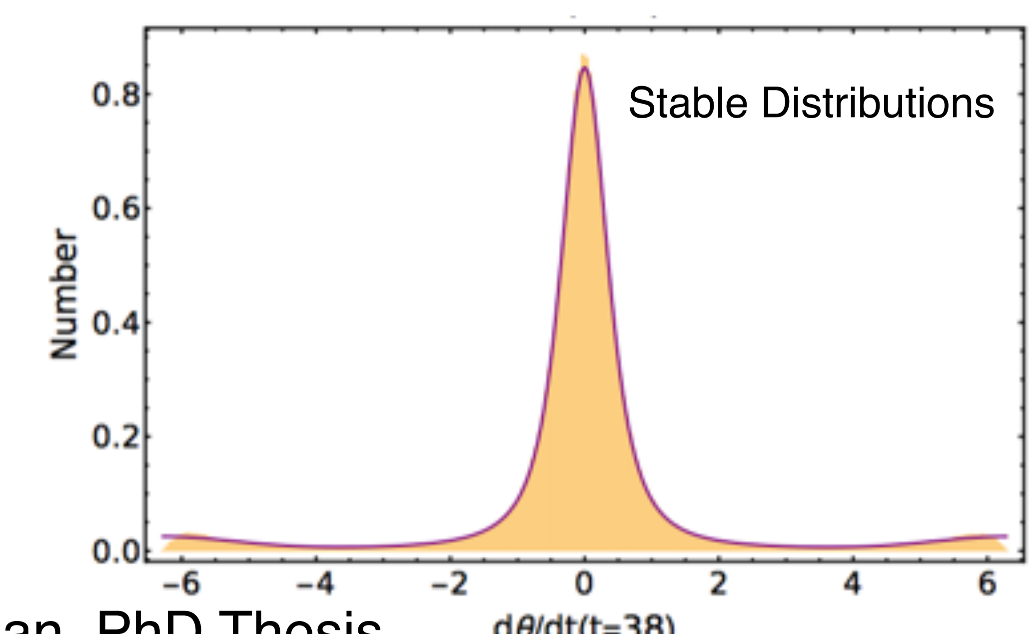




$$C(t) = e^{R(t)+i\theta(t)} \rightarrow \frac{1}{N}\sum_{U_i} e^{R(t;U_i)+i\theta(t;U_i)}$$

$$\langle C(t)\rangle \approx \left\langle e^{R(t)}\right\rangle \left\langle e^{i\theta(t)}\right\rangle \sim \left(e^{-\frac{3}{2}m_\pi t}\right)\left(e^{-(m_N-\frac{3}{2}m_\pi)t}\right)$$





Michael Wagman, PhD Thesis

Quantum Field Theory Foundational Papers

Simulating lattice gauge theories on a quantum computer

Tim Byrnes[*]
National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan

Yoshihisa Yamamoto
E. L. Ginzton Laboratory, Stanford University, Stanford, CA 94305 and National Institute of Informatics, 2-1-2 Hitotsubashi, Chiyoda-ku, Tokyo 101-8430, Japan
(Dated: February 1, 2008)

We examine the problem of simulating lattice gauge theories on a universal quantum computer. The basic strategy of our approach is to transcribe lattice gauge theories in the Hamiltonian formulation into a Hamiltonian involving only Pauli spin operators such that the simulation can be performed on a quantum computer using only one and two qubit manipulations. We examine three models, the U(1), SU(2), and SU(3) lattice gauge theories which are transcribed into a spin Hamiltonian up to a cutoff in the Hilbert space of the gauge fields on the lattice. The number of qubits required for storing a particular state is found to have a linear dependence with the total number of lattice sites. The number of qubit operations required for performing the time evolution corresponding to the Hamiltonian is found to be between a linear to quadratic function of the number of lattice sites, depending on the arrangement of qubits in the quantum computer. We remark that our results may also be easily generalized to higher SU(N) gauge theories.

Phys.Rev. A73 (2006) 022328

Quantum Computation of Scattering in Scalar Quantum Field Theories

Stephen P. Jordan,[†§] Keith S. M. Lee,[‡§] and John Preskill [§ *]

[†] *National Institute of Standards and Technology, Gaithersburg, MD 20899*
[‡] *University of Pittsburgh, Pittsburgh, PA 15260*
[§] *California Institute of Technology, Pasadena, CA 91125*

Abstract

Quantum field theory provides the framework for the most fundamental physical theories to be confirmed experimentally, and has enabled predictions of unprecedented precision. However, calculations of physical observables often require great computational complexity and can generally be performed only when the interaction strength is weak. A full understanding of the foundations and rich consequences of quantum field theory remains an outstanding challenge. We develop a quantum algorithm to compute relativistic scattering amplitudes in massive ϕ^4 theory in spacetime of four and fewer dimensions. The algorithm runs in a time that is polynomial in the number of particles, their energy, and the desired precision, and applies at both weak and strong coupling. Thus, it offers exponential speedup over existing classical methods at high precision or strong coupling.

Quantum Information and Computation 14, 1014-1080 (2014)

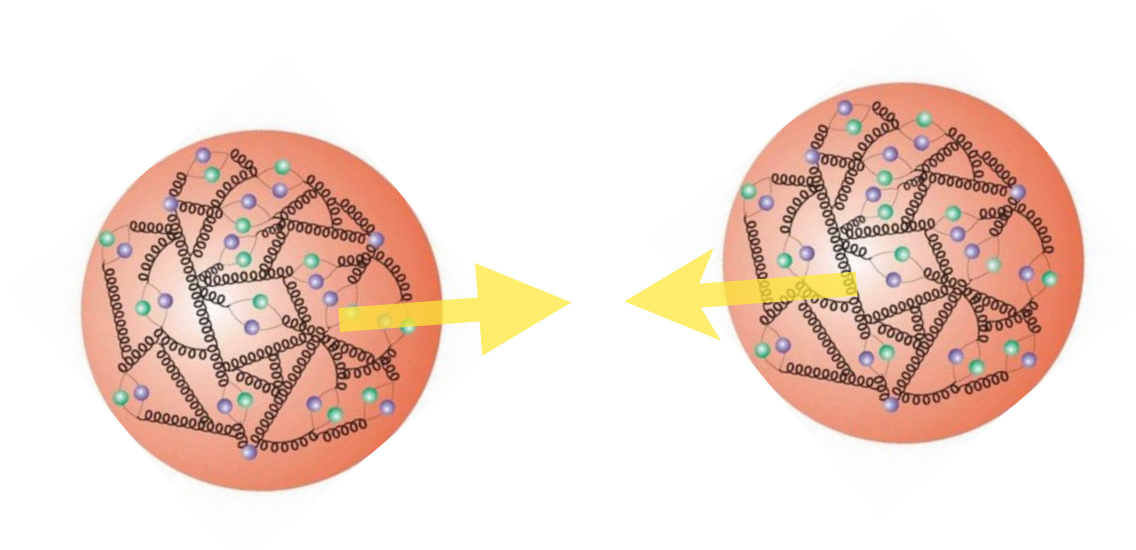
Detailed formalism for 3+1 Hamiltonian Gauge Theory

Discretrized spatial volume - no quarks

10^4 spatial lattice sites would require 10^5 * D qubits ,
D=size of register defining value of the field

Scalar Field Theory - Hamiltonian is nice

Quantum Chromodynamics
Asymptotic States



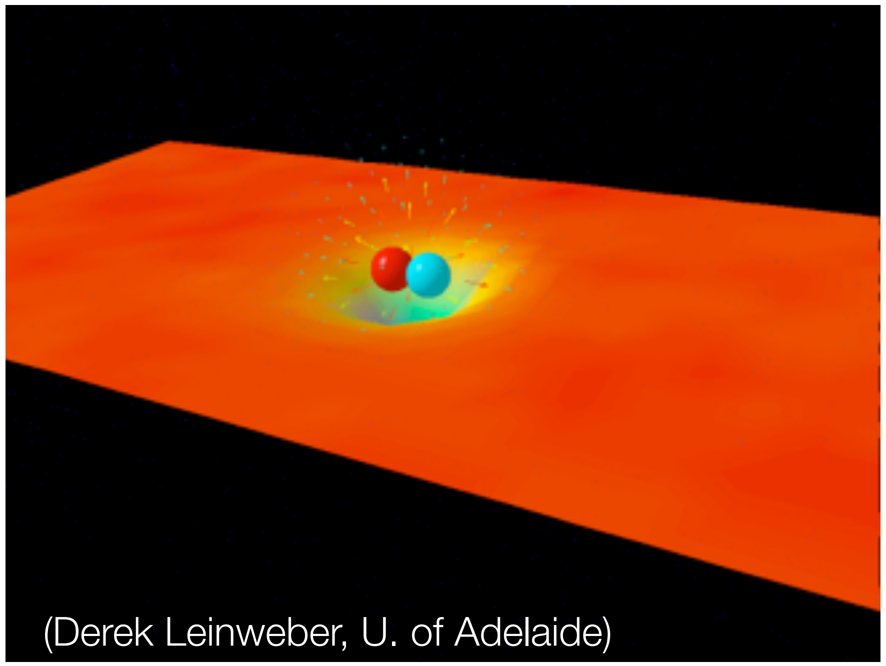
- Asymptotic states of QCD are nonperturbative states of quarks and gluons, and the strong vacuum itself is condensate of quarks and gluons that breaks (approximate) global symmetries of QCD.

- Hamiltonian or not or both?   Parallel Integrator ?

- Maybe start with recovering energy-eigenvalues, and S-matrix elements ala Luscher - classical computing provides optimal spatial sources/sinks ?

- Initialization of QC registers - what is the mapping of the problem?

QCD Hamiltonian on a Spatial Lattice


(Derek Leinweber, U. of Adelaide)

One way to tackle this, might not be the only or best way

$$\boldsymbol{H}_{\mathrm{SU(3)}} = \sum_{r,\mu}\sum_{\alpha=1}^{8} \left(\boldsymbol{E}^{\alpha}(r,\mu)\right)^2 - x \sum_{p\in\{\mathrm{plaquettes}\}} \left(\boldsymbol{Z}(p) + \boldsymbol{Z}^{\dagger}(p)\right)$$

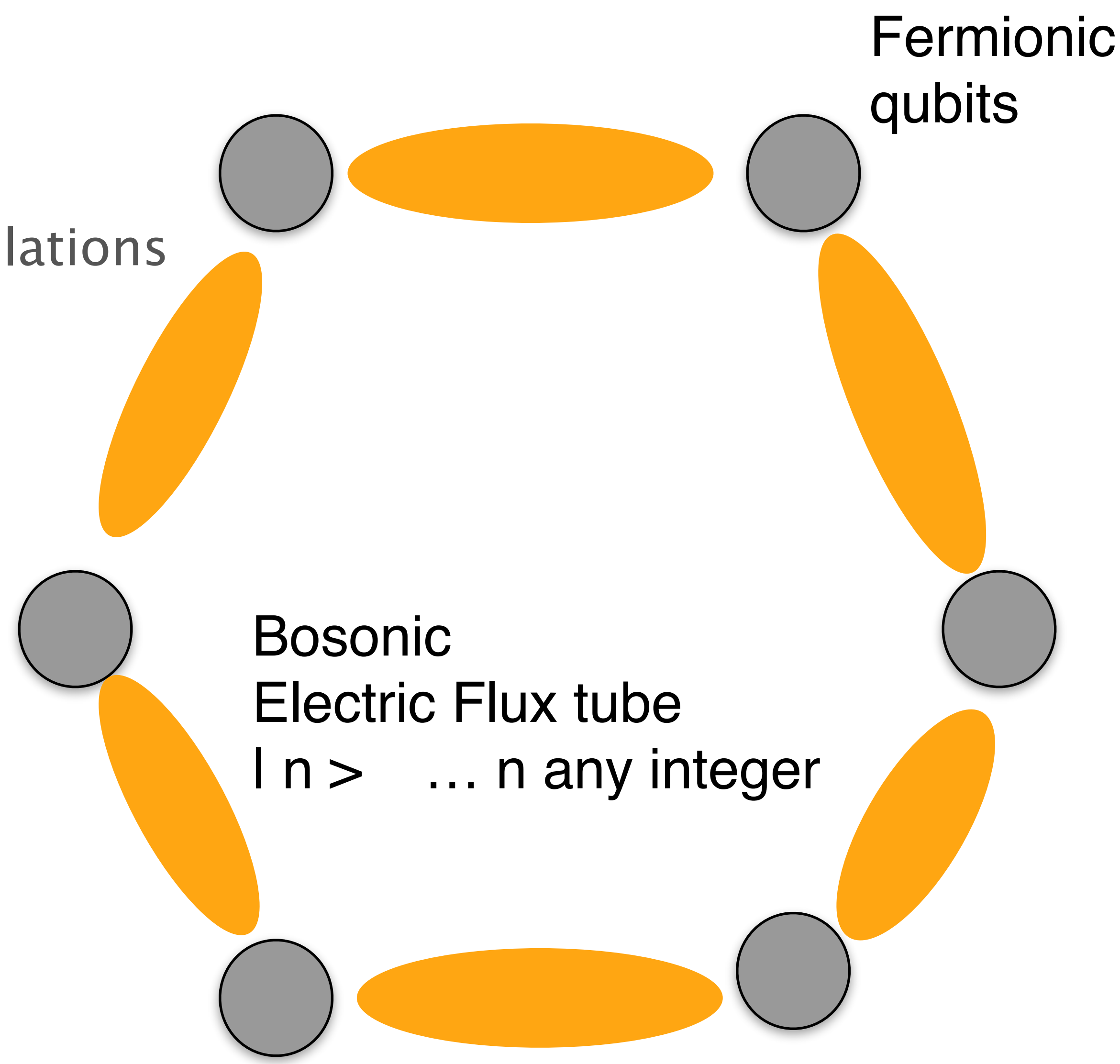
$$\hat{H}_W = \frac{1}{2}\sum_{\mathbf{x}} [\hat{\psi}^{\dagger}_{\mathbf{x}}, \gamma^0\Big(-i\not{D}^s_W + m\Big)\hat{\psi}_{\mathbf{x}}].$$

$$-i\not{D}^s_W\hat{\psi}_{\mathbf{x}} = \frac{1}{2}\sum_{n,i} C_n\Big[\Big(-i\gamma^i - nr_w\Big)U_{\mathbf{x},+n\mathbf{i}}\hat{\psi}_{\mathbf{x}+n\mathbf{i}} + 2nr_w\hat{\psi}_{\mathbf{x}} - \Big(-i\gamma^i + nr_w\Big)U_{\mathbf{x},-n\mathbf{i}}\hat{\psi}_{\mathbf{x}-n\mathbf{i}}\Big]$$

+improvements in discretization (clover, etc)
+ or actions with good chiral symmetry

Schwinger Model - 1+1 Dim QED
A Playground for QCD

Heterogeneous Digital-Analog Quantum Dynamics Simulations



Two ORNL-led research teams receive $10.5 million to advance quantum computing for scientific applications

ORNL's Pavel Lougovski (left) and Raphael Pooser will lead research teams working to advance quantum computing for scientific applications. Credit: Oak Ridge National Laboratory, U.S. Dept. of Energy (hi-res image)

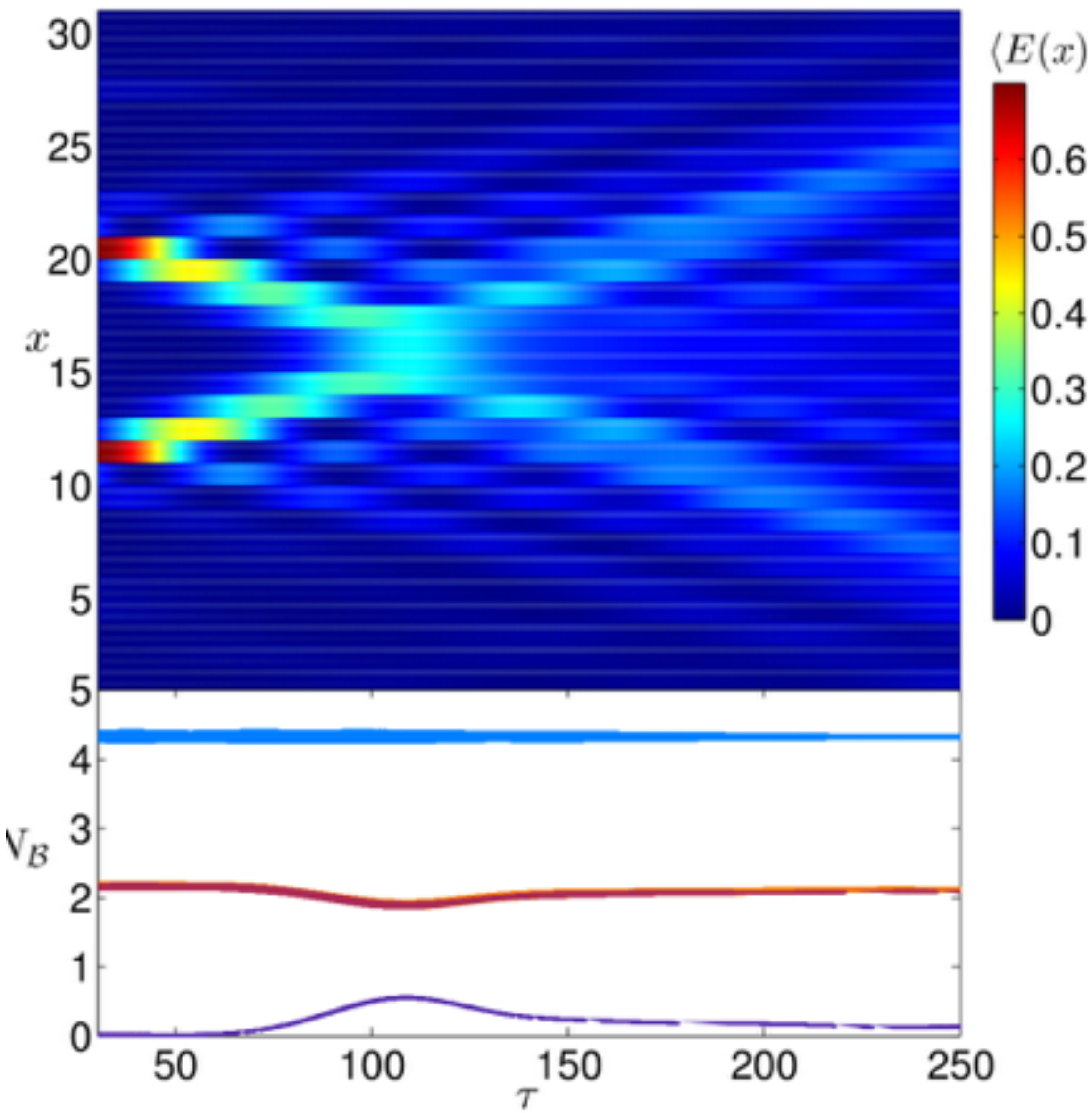
Confinement and condensate
Dualities in 1+1 dim
local and nearest neighbour interactions
PBCs or other (e.g., open)
strong coupling limit is anti-ferromagnetic ground state

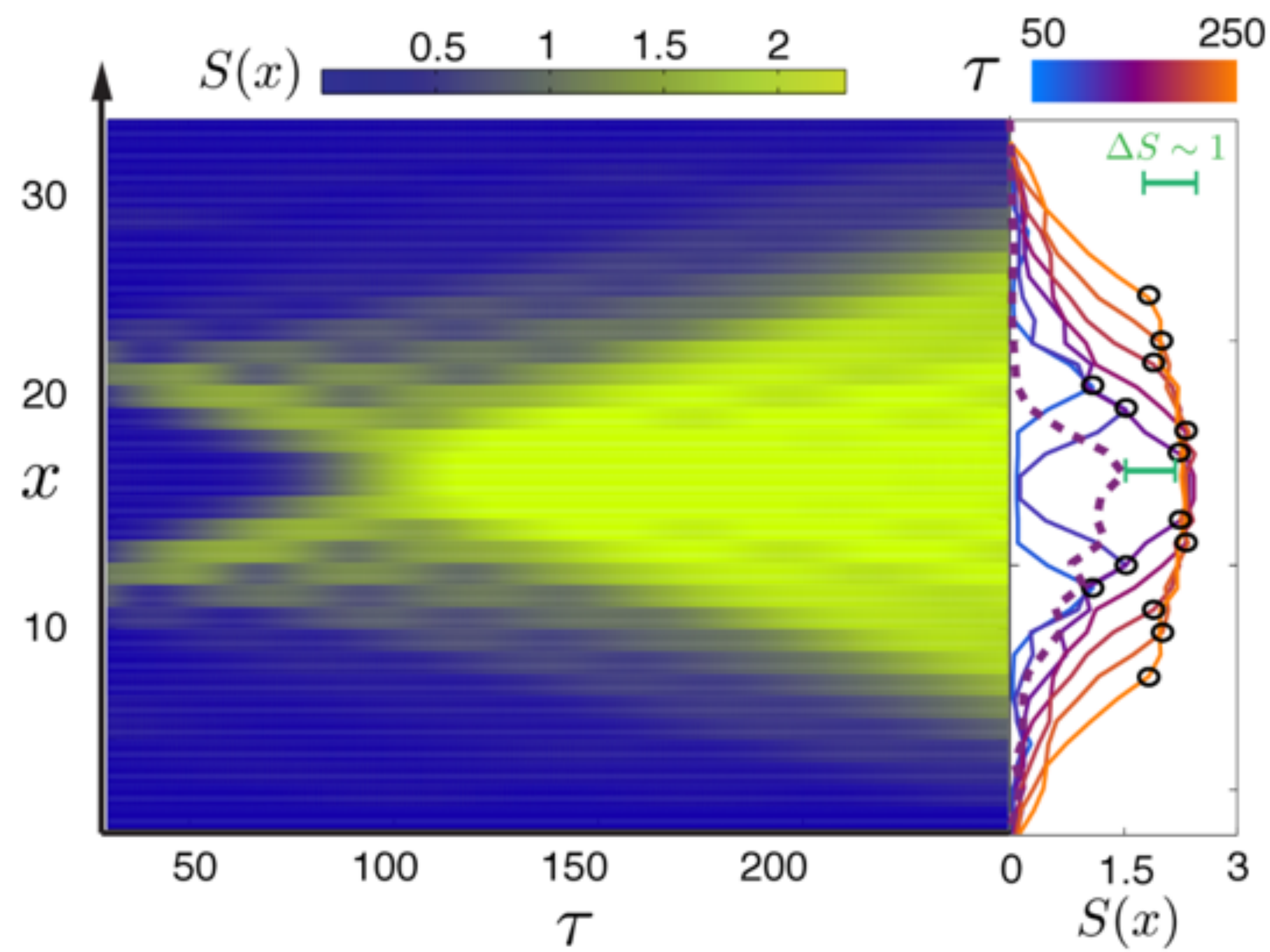
Schwinger Model - 1+1 Dim QED
Dynamics : Interactions

Real-time Dynamics in U(1) Lattice Gauge Theories with Tensor Networks

T. Pichler,[1] M. Dalmonte,[2,3] E. Rico,[4,5,6] P. Zoller,[2,3] and S. Montangero[1]

Phys. Rev. X **6**, 011023 – Published 3 March 2016





Schwinger Model - 1+1 Dim QED Construction

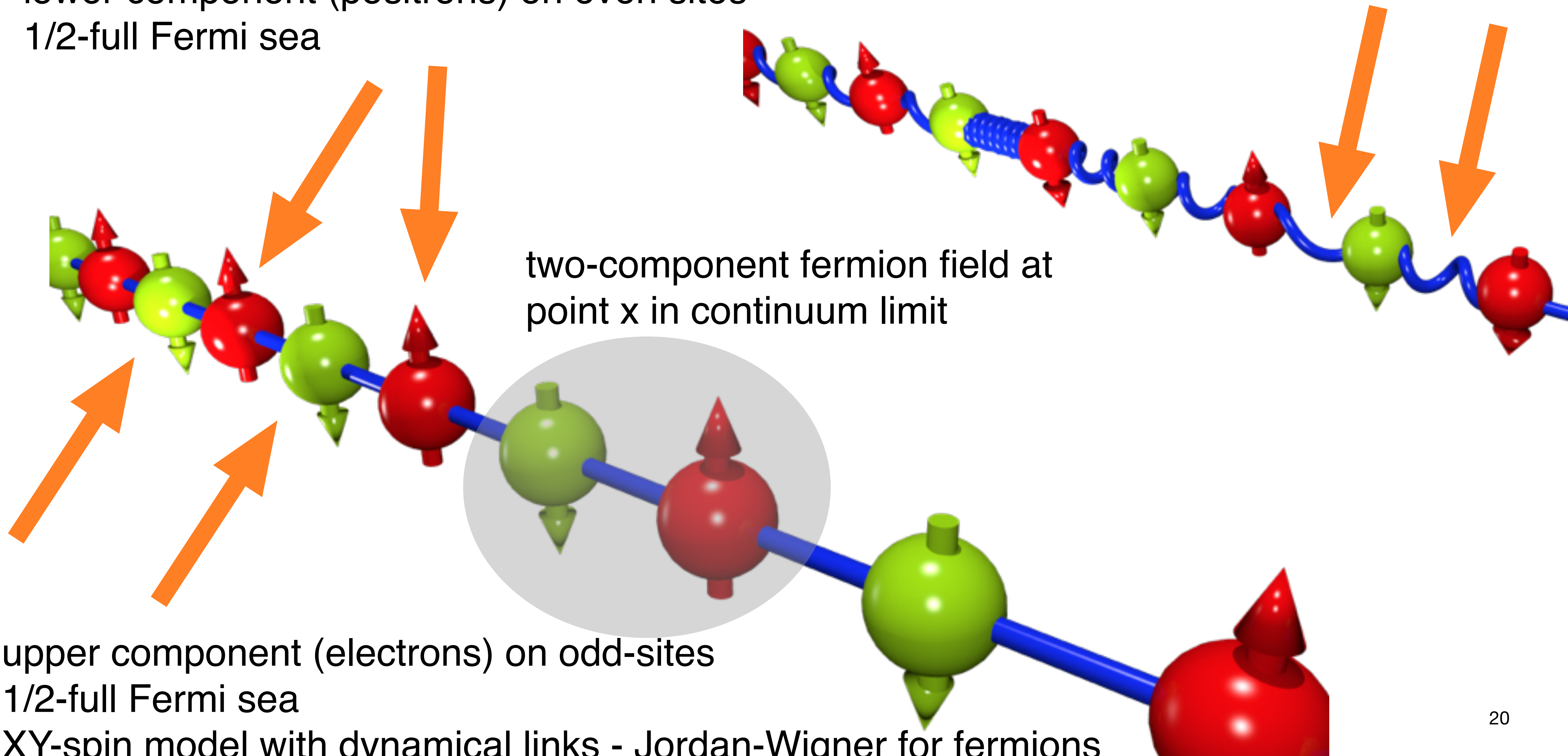
Natalie Klco and MJS

Staggered fermions - Kogut, Banks, Susskind early 1970's

excite electric field through pair creation and annhilation

lower component (positrons) on even sites
1/2-full Fermi sea

two-component fermion field at point x in continuum limit

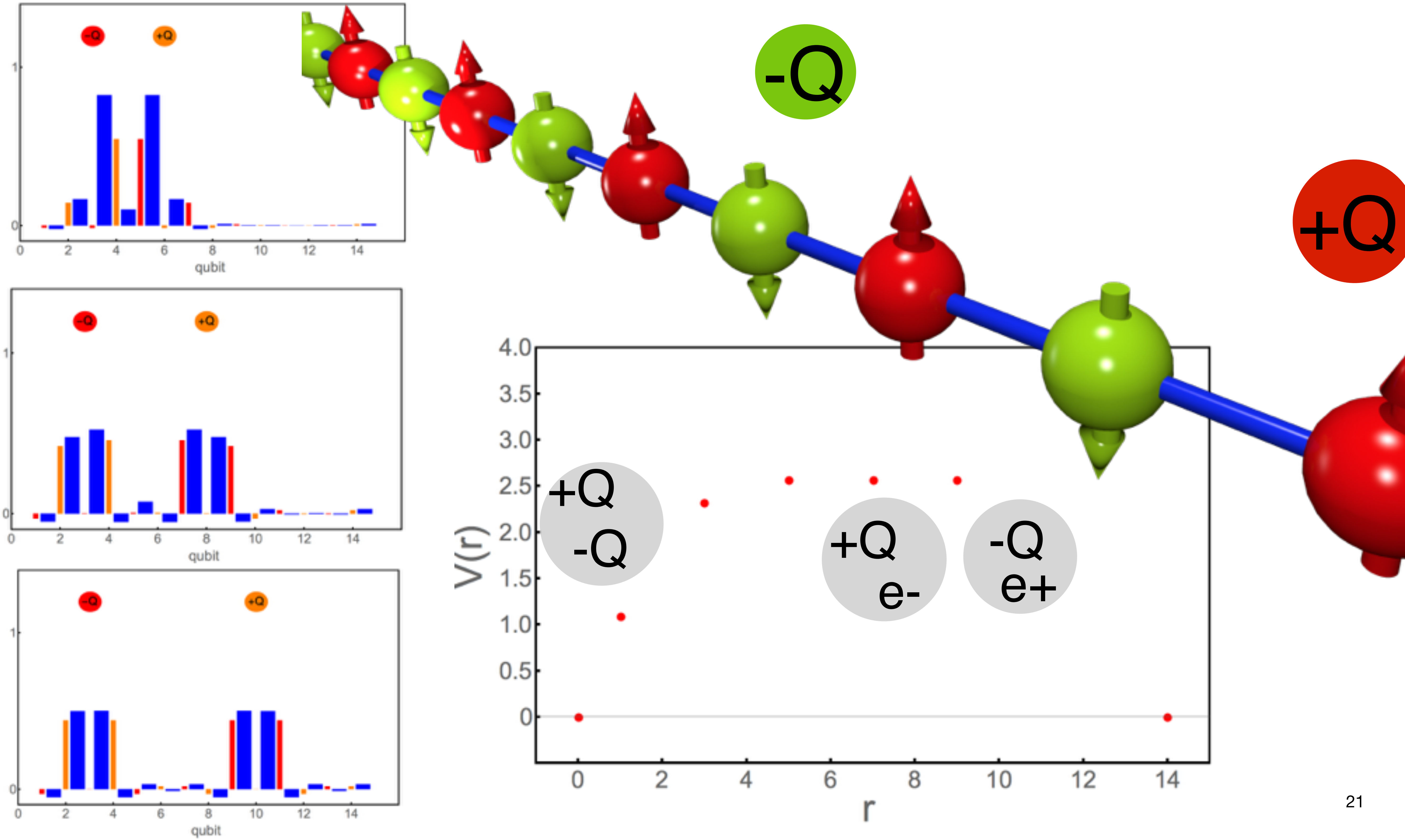


upper component (electrons) on odd-sites
1/2-full Fermi sea

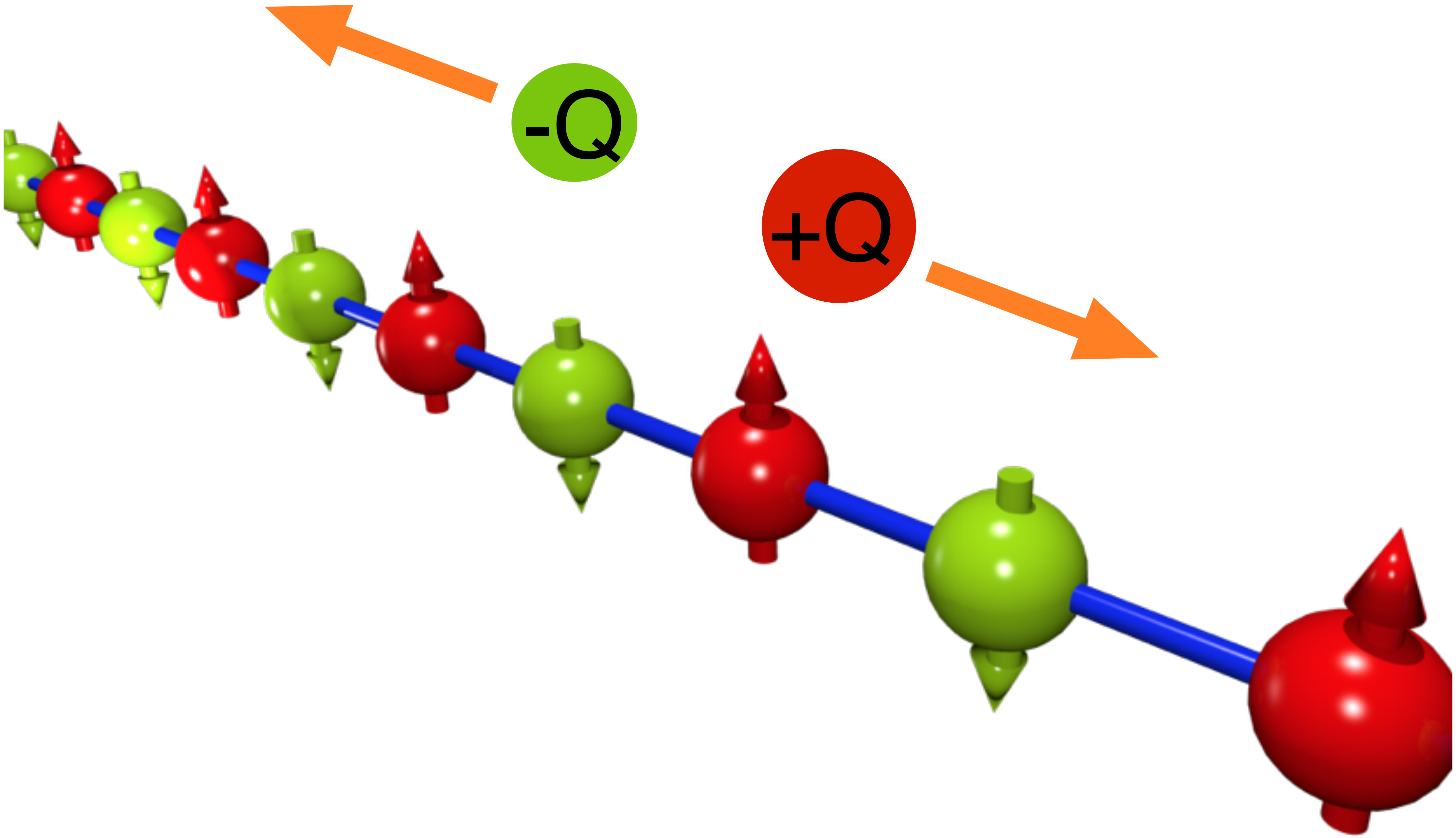
XY-spin model with dynamical links - Jordan-Wigner for fermions

Schwinger Model - 1+1 Dim QED
Charge Screening

Natalie Klco and MJS

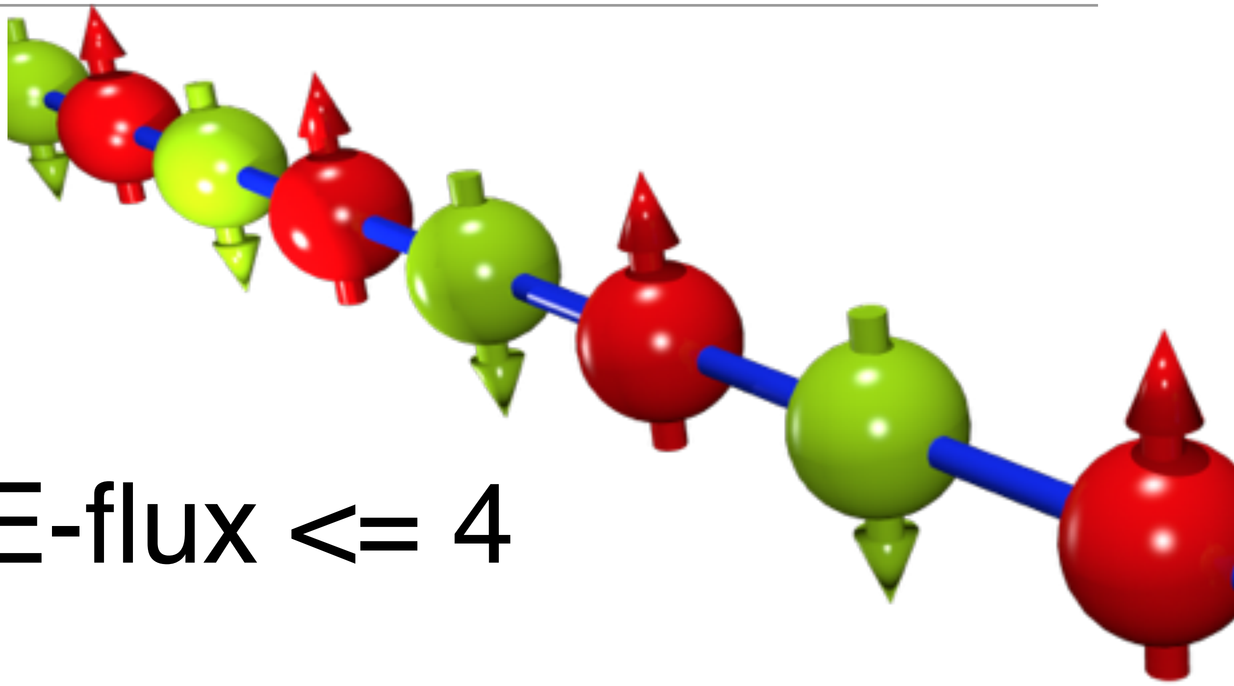


Schwinger Model - 1+1 Dim QED
Dynamics : Fragmentation Functions



Will require isolation of the low states
Source-independence will be critical to assess systematics - variational approaches

Schwinger Model - 1+1 Dim QED
States and Constraints



e.g., NQ = 14 and energy in E-flux <= 4

~ 10^{17} distinct states to consider

Gauss's Law - constrains adjacent links by charges on qubits AND retains only states connected to the anti-ferromagnetic state with empty links by H .

~ 10^{3} states

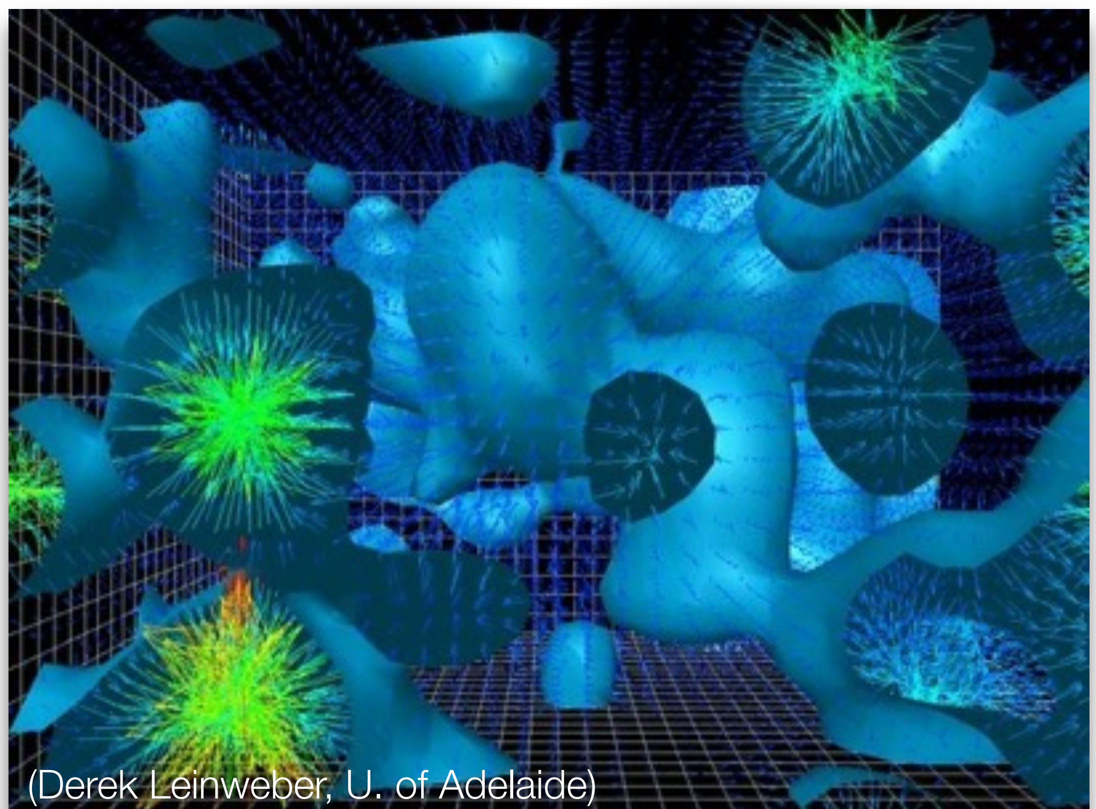
It is important to get the quantum vacuum right!

What is the Full QCD Vacuum : $E^a |0\rangle = 0$?

Random fields at each point in spacetime is far from ground state.

- generally all 0++ states will be populated with some amplitude

$|\text{random}\rangle = a|0\rangle + b|(\text{pi pi})\rangle + c|(\text{pi pi pi pi})\rangle + \ldots + d|(GG)\rangle + \ldots$



1 vacuum configuration

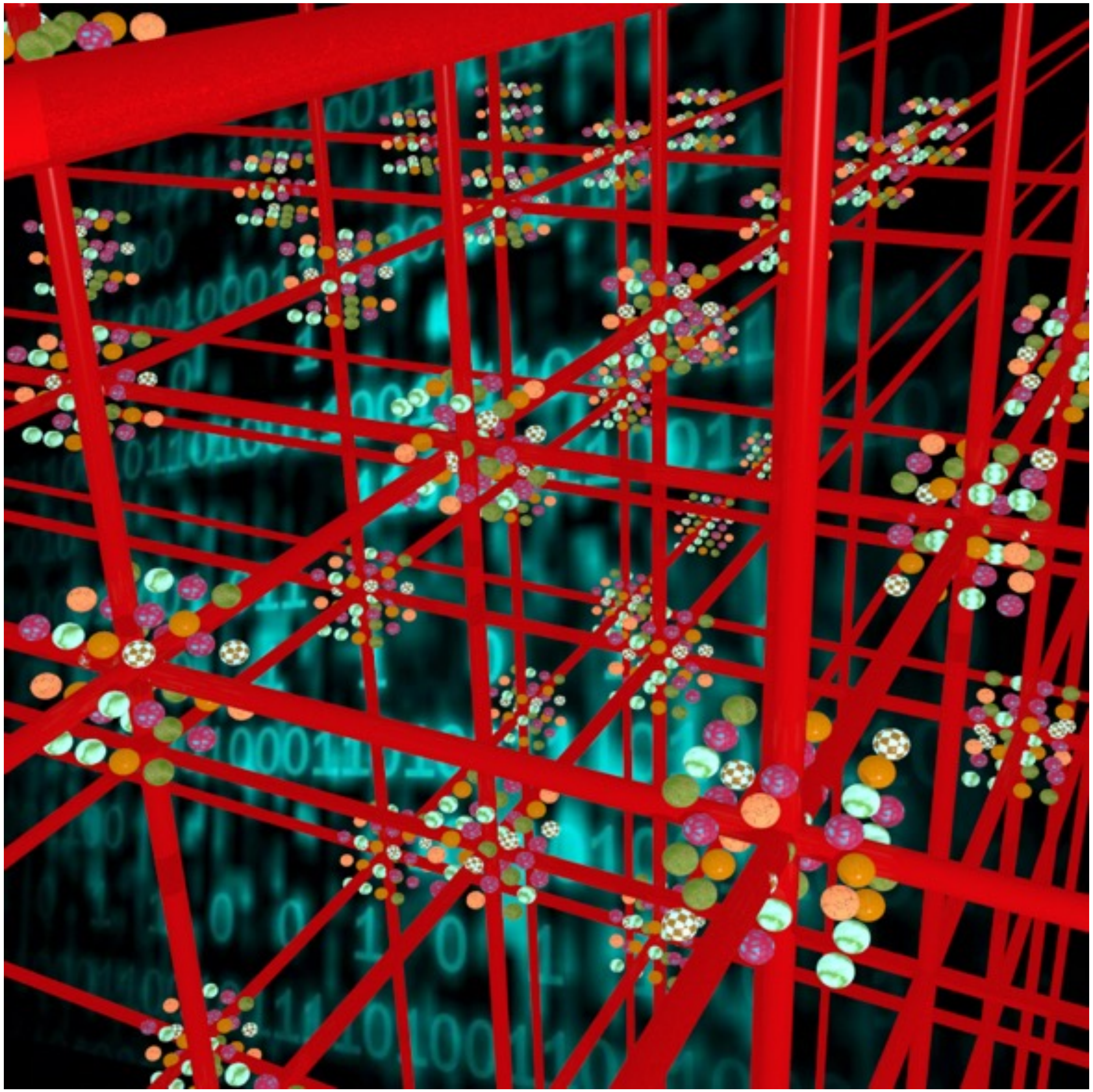
Probability $e^{-S_{QCD}}$

$|\text{random}\rangle$ needs to be ``cooled" to $|0\rangle$

In Lattice QCD, first 1000 steps of HMC thermalize

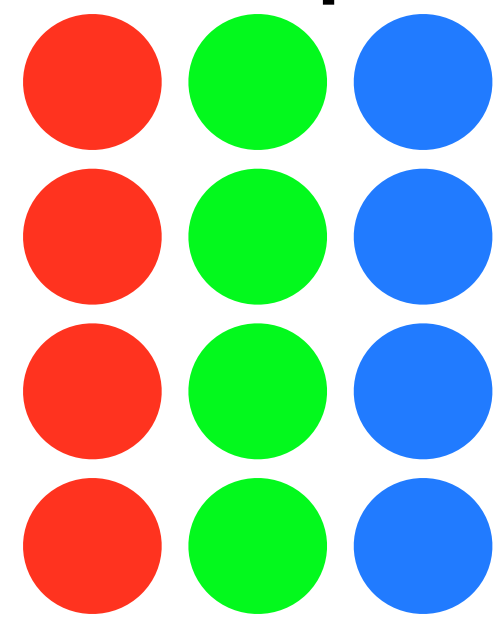
Euclidean-space Lattice QCD and QC might be profitable

QC for Hamiltonian QCD
Naive Estimates of System Register

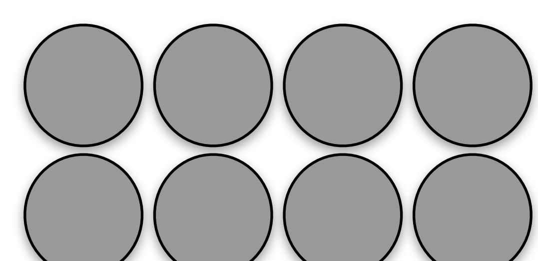


up-quark qubits

u_1
u_2
u_3
u_4



+ d,s,c



QC for Hamiltonian QCD
Naive Estimates of System Register

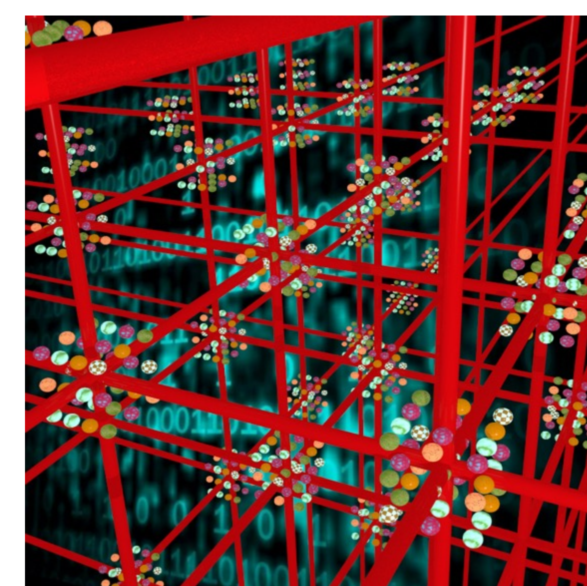
Each site has a register of qubits, scales with spatial volume

e.g., fully-dynamical QCD
u,d,s quarks
Number of Qubits $= 36\ L^3 + 24\ L^3\ n_{res}$

e.g., $L=10$ and $n_{res}=6$
Number of Qubits $= 180\ L^3 = 180K$

c/w: Quenched QCD
$L=10$ and $n_{res}=6$
Number of Qubits $= 24\ L^3\ n_{res} = 144K$

c/w: Scalar-field Theory:
$L=10$ and $n_{res}=6$
Number of Qubits $= L^3\ n_{res} = 6K$



Lattice spacing and volume extrapolations remain

Non-Abelian Gauge Theories

http://online.kitp.ucsb.edu/online/qcontrol-c13/zoller/pdf/Zoller_QControl13Conf_KITP.pdf

Towards Quantum Simulating QCD

(2014)

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Abstract

Quantum link models provide an alternative non-perturbative formulation of Abelian and non-Abelian lattice gauge theories. They are ideally suited for quantum simulation, for example, using ultracold atoms in an optical lattice. This holds the promise to address currently unsolvable problems, such as the real-time and high-density dynamics of strongly interacting matter, first in toy-model gauge theories, and ultimately in QCD.

Keywords: Quantum simulation, sign problem, real-time dynamics of gauge theories

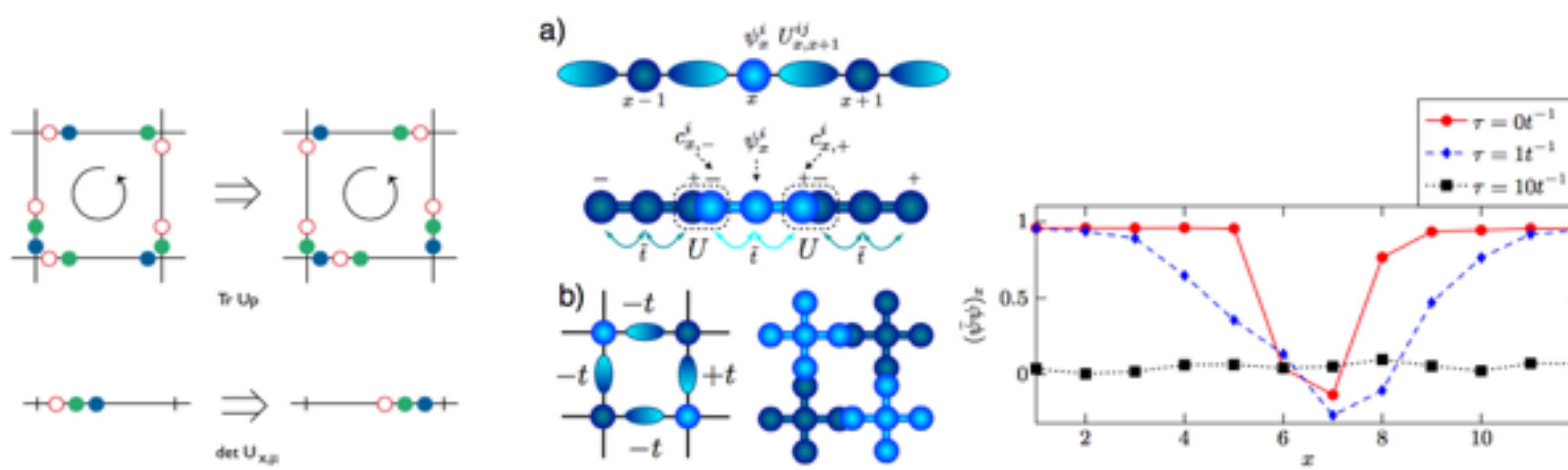


Figure 3. *Left: In an $SU(3)$ quantum link model, three fermionic rishons of different colors reside on each link. The Hamiltonian moves the rishons around plaquettes or along links, like the beads of an abacus. Middle: Quantum simulator for an $SU(N)$ gauge theory with ultracold alkaline-earth atoms representing "quarks" or rishon constituents of "gluons" in a 1-d (a) or 2-d (b) optical superlattice. Depending on its position in the optical lattice, an alkaline-earth atom either embodies a "quark" or a rishon. Gauge invariance is protected by the internal $SU(2I+1)$ symmetry of the nuclear spin I of the atoms. Right: Real-time τ evolution of the chiral order parameter profile $(\bar{\psi}\psi)_x$ in a $U(2)$ gauge theory, mimicking the expansion of a hot "quark-gluon" plasma [41].*

The Role of Quantum Computing for QCD in NP (circa 2017 !)

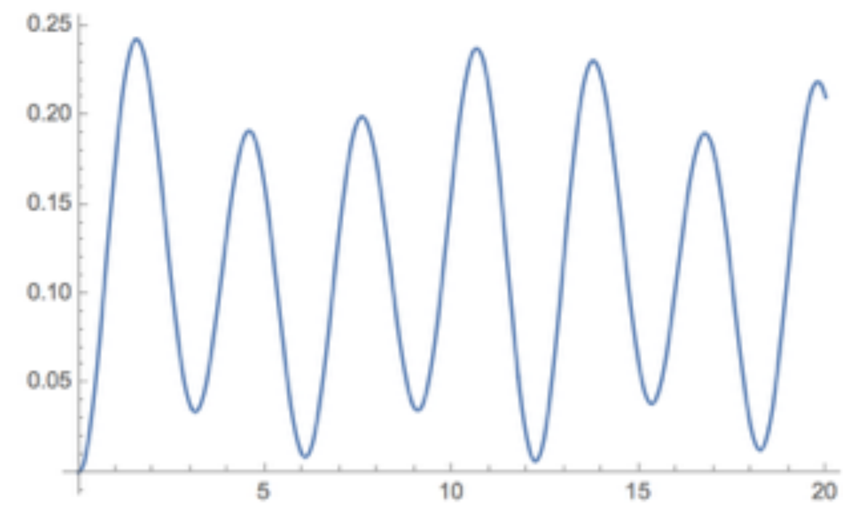
- Classical computing is on track to provide sufficient precision for many experimentally important quantities in HEP and NP in the Exascale.

- Finite density systems (including modest size nuclei) require exponentially challenging calculations that will likely benefit from QCs, or QCs+Exascale CCs.
  - QCs may be first used to accelerate parts of classical Lattice QCD calculations.

- Anticipate that Exascale classical systems will be required to ``precondition''/ map problem onto qubit registers of QC and then read from qubit registers - BUT currently little is known how to use a QC for QCD

Some Thoughts

1+1 dim Schwinger model (Pitchler, Martinez et al (2016), and others before)
- exciting and educational



At present, co-design seems essential - developing algorithms for present and near-term QC hardware, as opposed to ``fantasy/wishful thinking'' QC hardware.

Resource requirement estimates (qubits, gates, oracles) need to be for the integrated application - i.e. what will it actually take to accomplish the physics objective.

Physics understanding/techniques and algorithms for NP and HEP may be of benefit to more general QC objectives

INT/UW QC-QFT Initial Efforts

INSTITUTE for NUCLEAR THEORY

- Regular meetings of a group of ~7 people

- Valuable interactions with Microsoft Research
  - Nathan Weibe and/or Matthias Troyer every 2-3 of weeks
  - anticipate scientfic collaborations to emerge from our meetings
  - seminars/meetings at or arranged by Microsoft

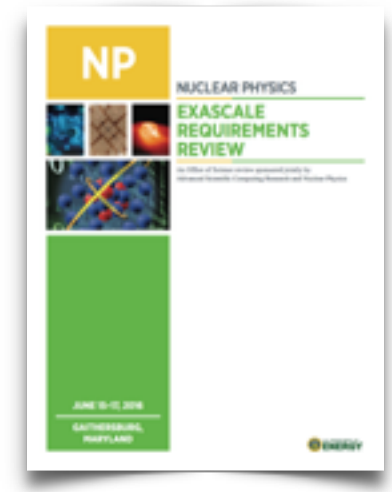
- Many-body and QFT
  - we are learning …
  - e.g., *Ground States via Spectral Combing on a Quantum Computer*,
    David B. Kaplan, Natalie Klco, Alessandro Roggero, arXiv:1709.08250 [quant-ph]

- Presently thinking about low-dimensional field theories with features similar to QCD

- Collaborating with ORNL's ``Heterogeneous'' project.

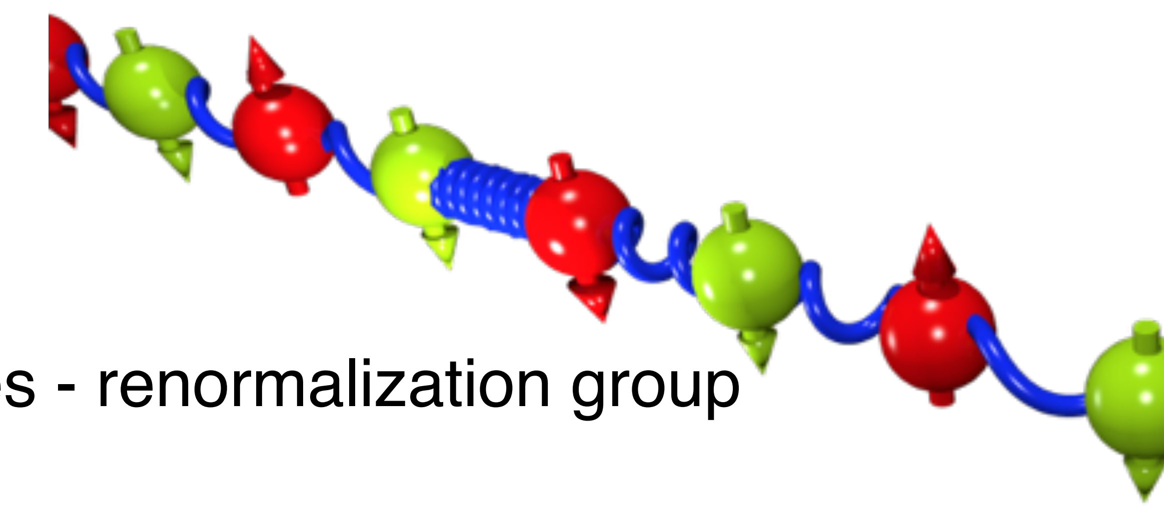
Summary

It is likely that QC will become significant in studies of quantum field theories and in achieving important objectives in Nuclear Physics.



A pyramid of classical HPC resources in the exascale will remain essential

- for physics production
- for preparing algorithms for quantum computers



- QC algorithms are required for QCD to address
  - systems of nucleons
  - finite density, chemical potentials
  - Hamiltonian evolution
  - Implementing low-energy effective field theories - renormalization group techniques, truncated Hilbert space techniques
- Collaborations with QC/QI experts to accomplish the science objectives
- Co-design important

- A modest SciDAC project would be beneficial, along with access to appropriate hardware and classical computing resources (``Quantum Quantum Algorithms" ??)