Quantum Simulation of quantum field theory in the light-front formulation

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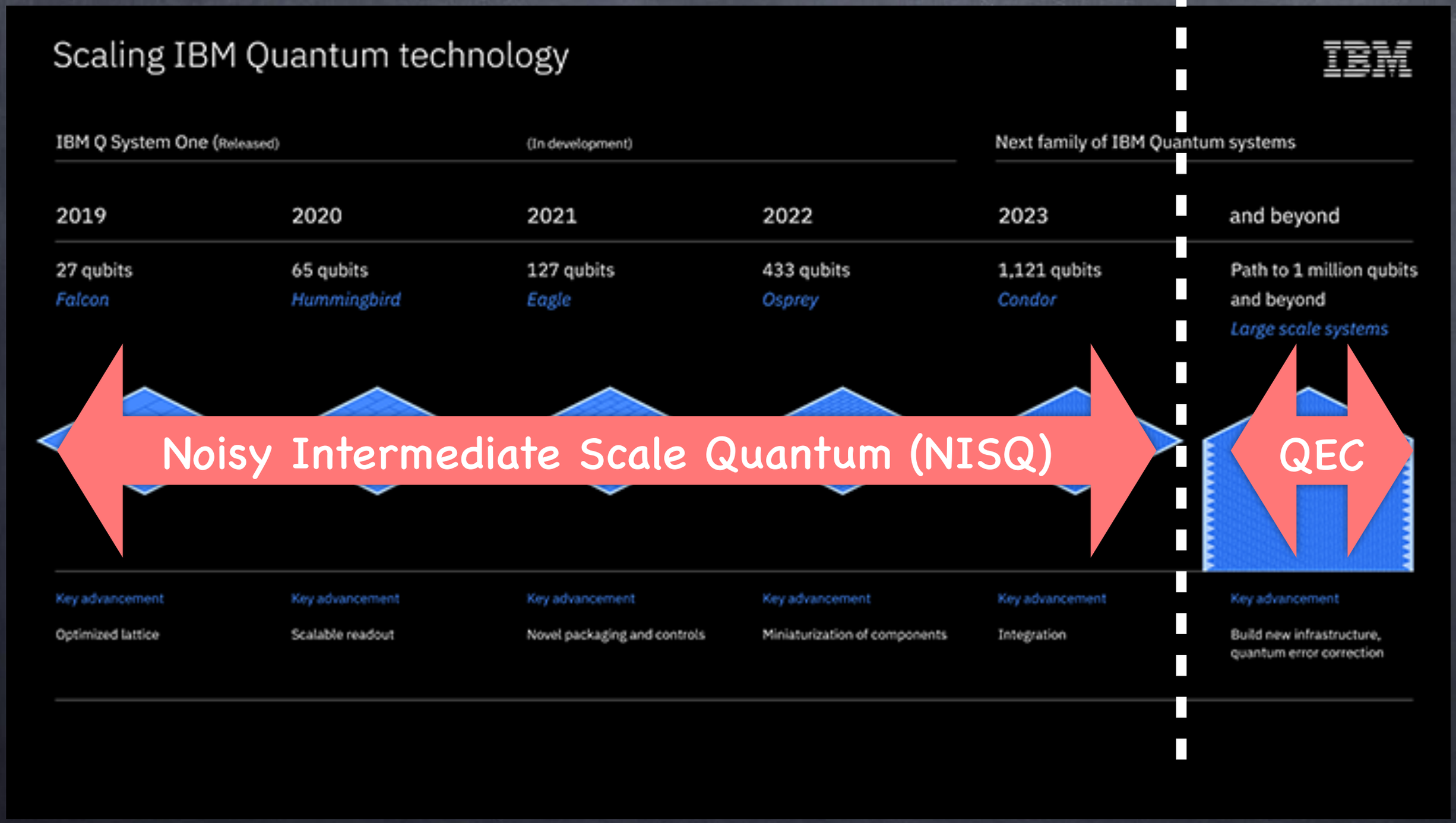
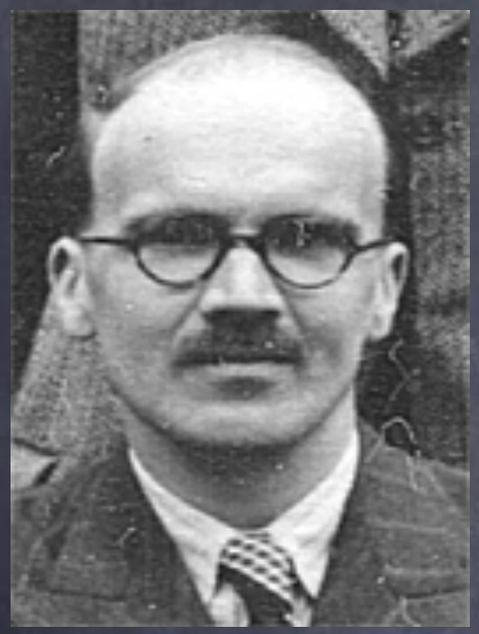
3 Brookhaven National Laboratory

NISQ and beyond: quantum computing with and without quantum error correction



https://www.ibm.com/blogs/research/2020/09/ibm-quantum-roadmap/

A Quantum Computer for Chemistry?



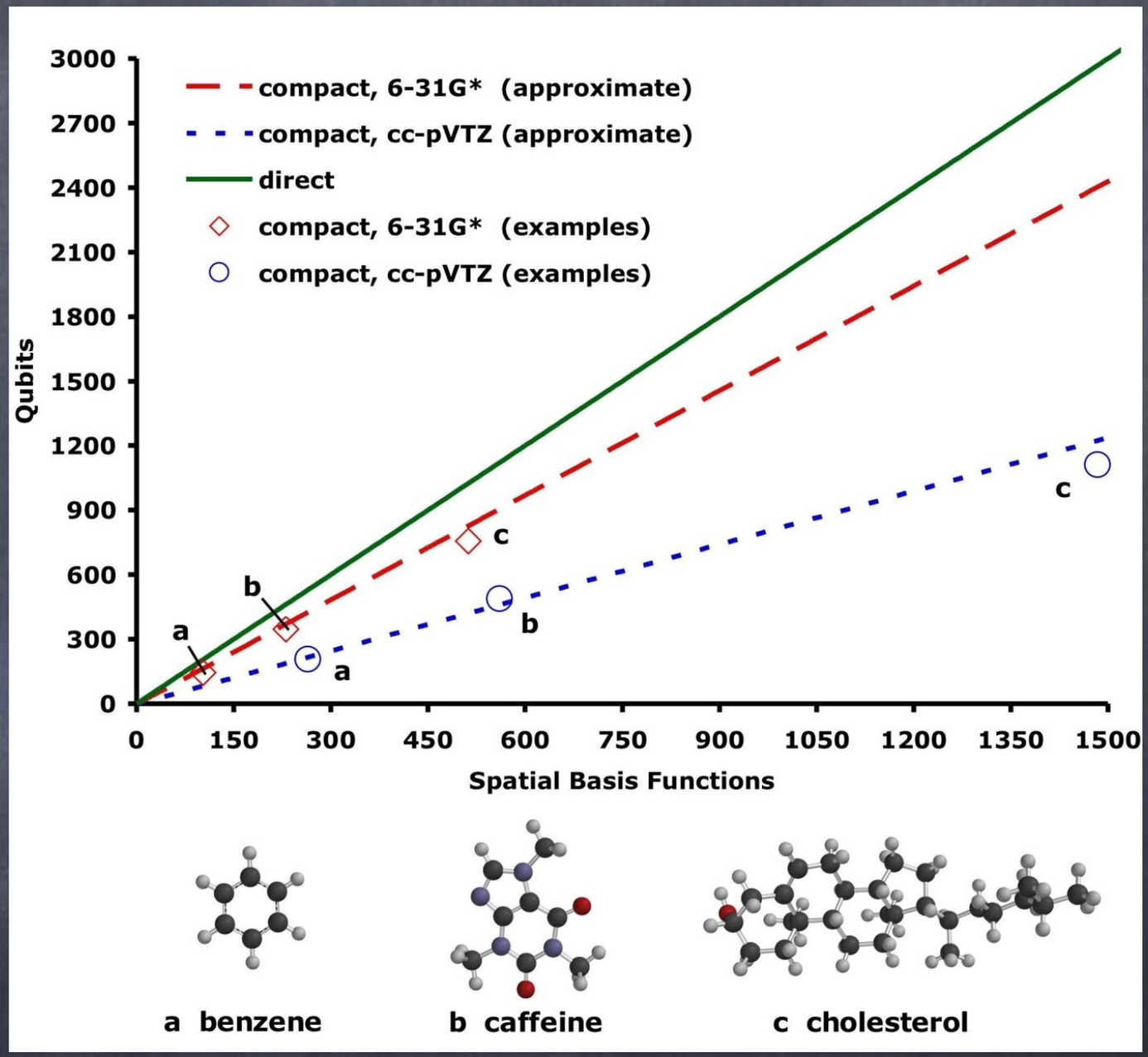
Electronic wave functions

II. A calculation for the ground state of the beryllium atom

By S. F. Boys, *Theoretical Chemistry Department, University of Cambridge**

(*Communicated by Sir Alfred Egerton, F.R.S.—Received* 31 *August* 1949)

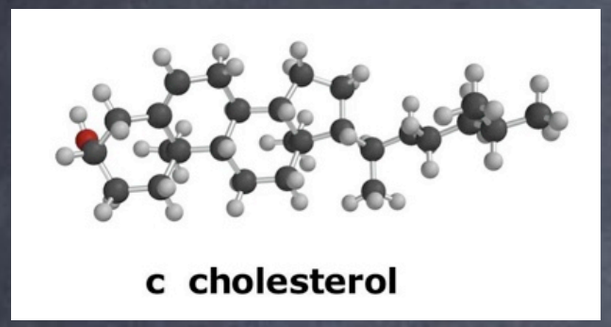
An approximate wave function expressed in terms of exponential functions, spherical harmonics, etc., with numerical coefficients has been calculated for the ground state of the beryllium atom. Judged by the energy criterion this gives a more accurate result than the Hartree result which was the best previously known. This has been calculated as a trial of a fresh method of calculating atomic wave functions. A linear combination of Slater determinants is treated by the variational method. The results suggest that this will provide a more powerful and convenient method than has previously been available for atoms with more than two electrons.



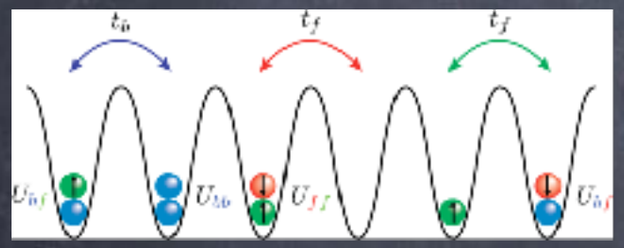
Simulated Quantum Computation of Molecular Energies, Alan Aspuru-Guzik, Anthony Dutoi, Peter J. Love, Martin Head-Gordon, Science, 309, 5741, (2005)

Simulating Fermions on a Quantum Computer

Molecules



Fermi-Hubbard Model



Map fermions to Qubits

State preparation

Phase estimation

Digital readout

E=??

Simulated Quantum Computation of Molecular Energies, Alan Aspuru-Guzik, Anthony Dutoi, **Peter J. Love**, Martin Head-Gordon, Science, **309**, 5741, (2005)

Two ways to simulate time evolution

Given a Hamiltonian: $H = \sum_{k=1}^{m} H_k$

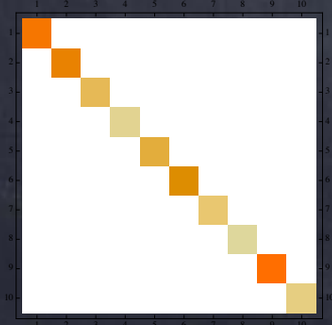
Two natural ideas of an "easy" Hamiltonian:

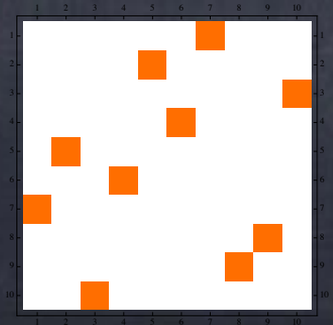
1) Terms are local (Direct Mappings)

Two-Local $H = \sum_{i,j} c_{ij} X_i \otimes X_j$

Three-Local $H = \sum_{i,j} c_{ijk} X_i \otimes Y_j \otimes Z_k$

2) Terms are sparse (Compact Mappings)





NISQ applications - Variational Algorithms

Ansatz quantum circuit U

Q

Samples

C

Samples

01010100010
10001001000
10001001001

Expectation value

Peruzzo, et al Nature Communications, 5:4213, (2014), Farhi et al. arXiv:1411.4028 [quant-ph]

Variational Quantum Eigensolver - VQE

We want to find the smallest eigenvalue of:

$$H = \sum_{P_i \in S} \alpha_i P_i$$

Variationally minimize:

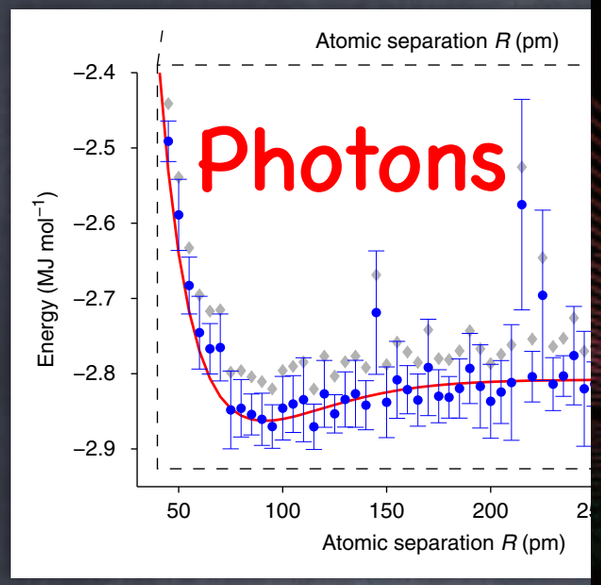
$$\langle H \rangle = \sum_{P_i \in S} \alpha_i \langle P_i \rangle$$

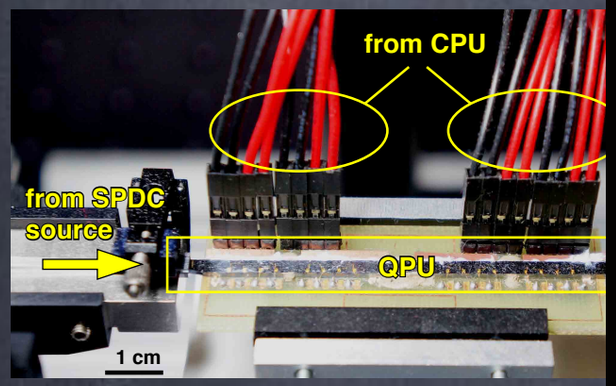
Classically separate minimization of each term fails - rdms do not correspond to global state

Quantumly one can variationally minimize a global quantum state, evaluate terms separately

A variational eigenvalue solver on a quantum processor Peruzzo, et al Nature communications 5 (4213), (2014),
Scalable Quantum Simulation of Molecular Energies, O'Malley et al. Physical Review X 6 (3), 031007,
Quantum chemistry calculations on a trapped-ion quantum simulator, Hempel et al, http://arxiv.org/abs/1803.10238

Nasty, brutish and short: VQE on NISQ devices





A variational eigenvalue solve
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Scalable Quantum Simulation
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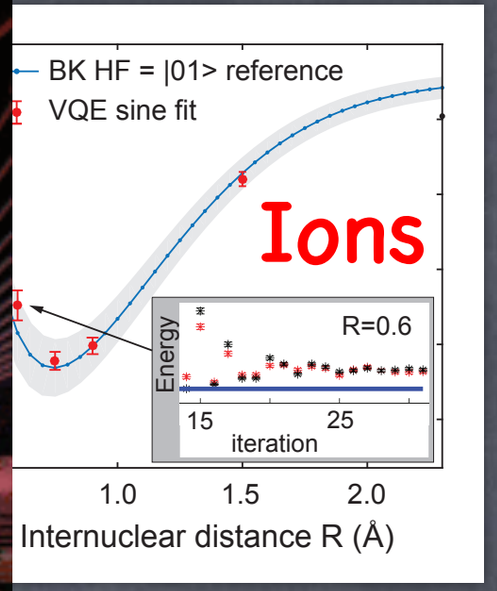
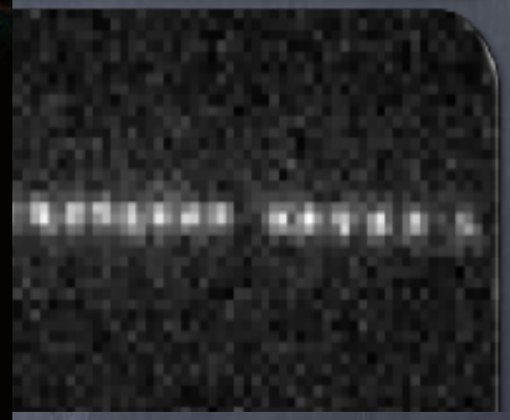
X 6 (3), 031007, (2016)





m chemistry calculations
apped-ion quantum
or, Hempel et al, Phys. Rev.
1022 (2018)

re-efficient variational
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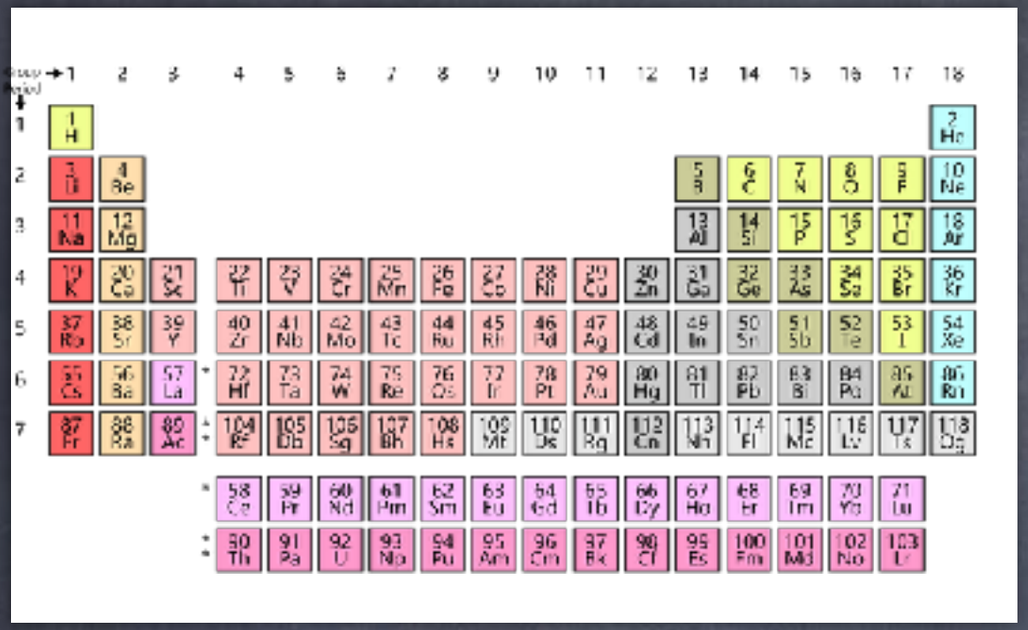
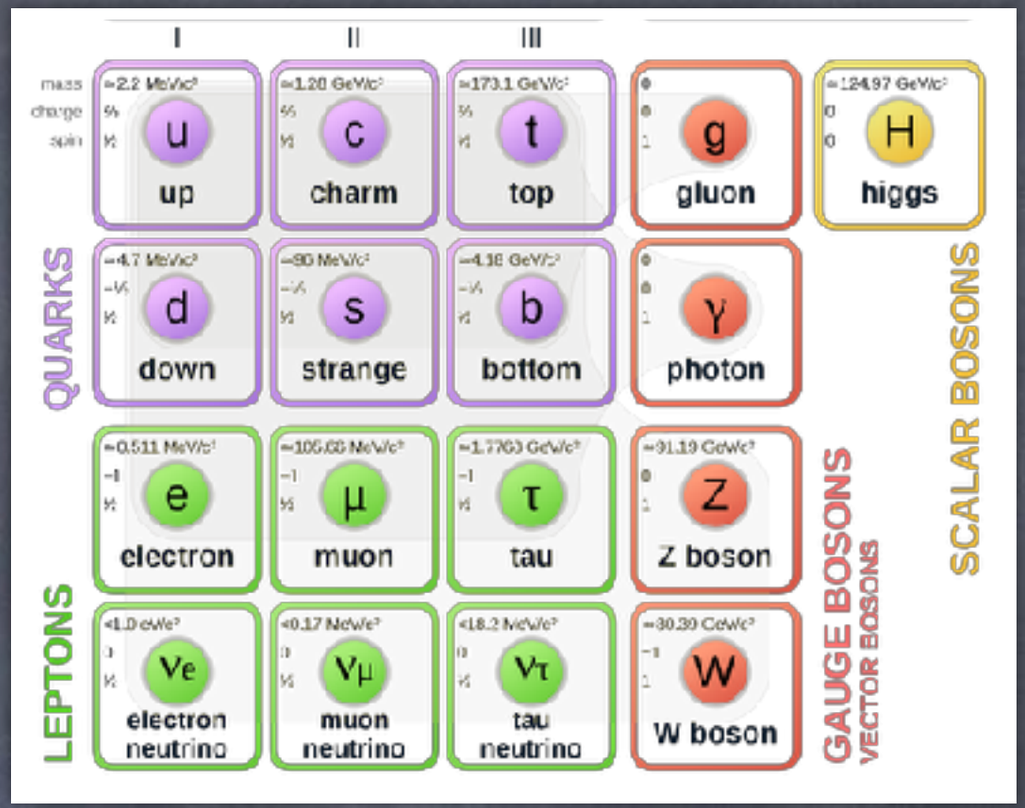
es and quantum magnets,
Kandala et al., Nature 549, pages
242–246 (2017)

From Quantum Chemistry to Quantum Field Theory





Fixed particle number

No sensible relativistic theory with fixed particle number

Basis representations requiring tens to hundreds of (logical) qubits

Use a grid as a regulator - discretize field values. Need ~thousands of qubits

Static properties

Scattering cross sections

Encoding Electronic Spectra in Quantum Circuits with Linear T Complexity, R Babbush, C Gidney, D Berry, N Wiebe, J McClean, A Paler, A Fowler, Hartmut Neven Physical Review X 8 (4), 041015, (2018)

RESEARCH ARTICLE

Quantum Algorithms for Quantum Field Theories

Stephen P. Jordan,[1]* Keith S. M. Lee,[2] John Preskill[3]

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Available online at www.sciencedirect.com

ScienceDirect

Nuclear Physics A 00 (2018) 1–8

Nuclear Physics A

Towards Quantum Simulating QCD

Uwe-Jens Wiese

Albert Einstein Center for Fundamental Physics, Institute for Theoretical Physics, Bern University, Sidlerstrasse 5, 3012 Bern, Switzerland

Two approaches:

1) Discretize field config. and represent directly.

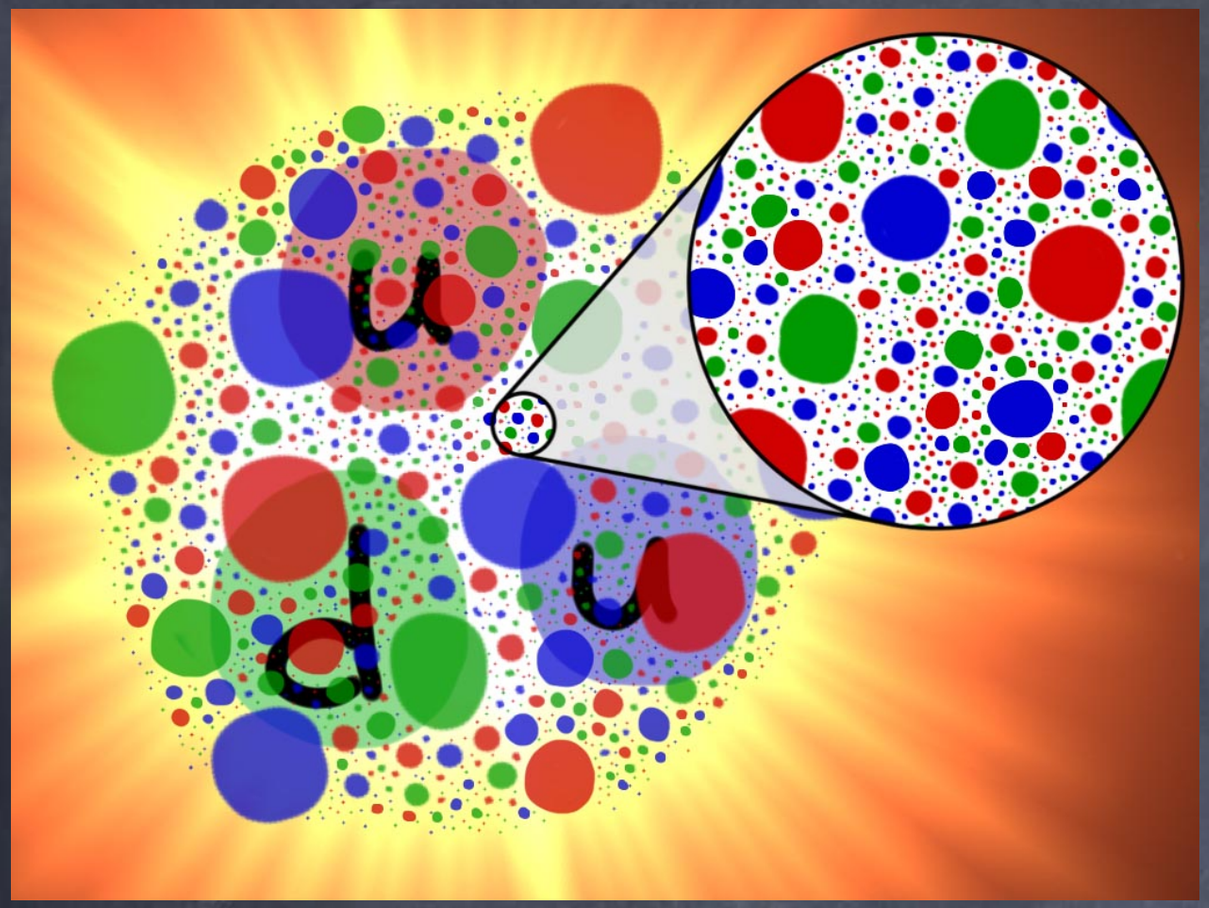
2) Quantum link models: discrete gauge variables, integrate out gauge fields, simulate complex spin model.

Daunting: 20^3 grid for 3+1 QCD: 400000 qubits.

Towards quantum simulating QCD, Uwe-Jens Wiese, Nucl. Phys. A 00 (2018) 1-8

Quantum algorithms for quantum field theories, S. P. Jordan, K. S. Lee, J. Preskill, Science 336, 1130-1133, (2012)

Static observable in QCD - the parton distribution function



LHC collides protons - composite particles

Momentum distribution of constituents captured by the parton distribution function (PDF).

Uncertainty in PDF can dominate.

Parton physics on a quantum computer H. Lamm, S. Lawrence, Y. Yamauchii arXiv:1908.10439 (2019)
Deeply inelastic scattering structure functions on a hybrid quantum computer, N. Mueller, A. Tarasov, and R. Venugopalan Phys. Rev. D 102, 016007
Computing real time correlation functions on a hybrid classical/quantum computer N Mueller, A Tarasov, R Venugopalan

The Light Front formulation

"Ab initio quantum chemistry is an emerging computational area that is fifty years ahead of lattice gauge theory, a principal competitor for supercomputer time, and a rich source of new ideas and new approaches to the computation of many fermion systems." Ken Wilson, 1990

x,t goes to x+ct, x-ct. P,E goes to P+E, P-E

Vacuum trivial

Orbital Basis Formulation

Makes QFT look like quantum chemistry

Good for quantum computation? Let's see!

Rev. Mod. Phys., 21:392-399, Jul 1949. Nuclear Physics B-Proceedings Supplements, 17:82-92, 1990.

REVIEWS OF MODERN PHYSICS VOLUME 21, NUMBER 3 JULY, 1949

Forms of Relativistic Dynamics

P. A. M. DIRAC
St. John's College, Cambridge, England

For the purposes of atomic theory it is necessary to combine the restricted principle of relativity with the Hamiltonian formulation of dynamics. This combination leads to the appearance of ten fundamental quantities for each dynamical system, namely the total energy, the total momentum and the 6-vector which has three components equal to the total angular momentum. The usual form of dynamics expresses everything in terms of dynamical variables at one instant of time, which results in specially simple expressions for six or these ten, namely the components of momentum and of angular momentum. There are other forms for relativistic dynamics in which others of the ten are specially simple, corresponding to various sub-groups of the inhomogeneous Lorentz group. These forms are investigated and applied to a system of particles in interaction and to the electromagnetic field.

Two requirements of fundamental theory:

1) Relativistic invariance

3) Hamiltonian formulation

1) implies coordinate systems related by Lorentz invariance are equivalent.

REVIEWS OF MODERN PHYSICS VOLUME 21, NUMBER 3 JULY, 1949

Forms of Relativistic Dynamics

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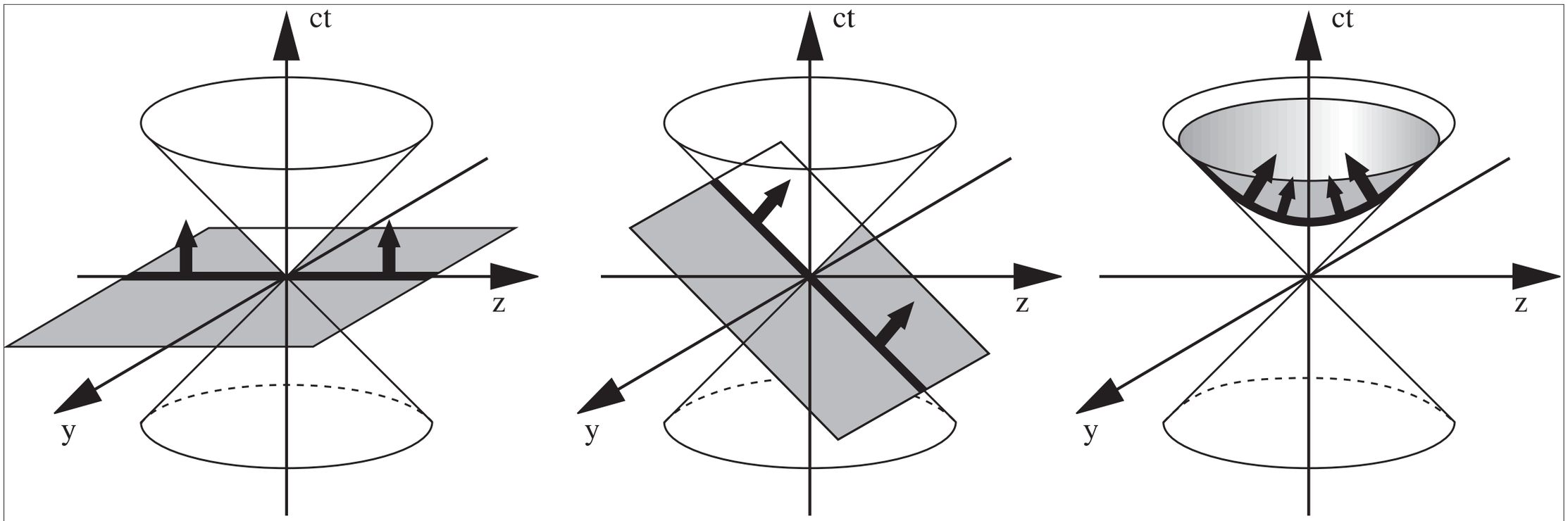


The instant form

$$\tilde{x}^0 = ct$$
$$\tilde{x}^1 = x$$
$$\tilde{x}^2 = y$$
$$\tilde{x}^3 = z$$

The front form

$$\tilde{x}^0 = ct + z$$
$$\tilde{x}^1 = x$$
$$\tilde{x}^2 = y$$
$$\tilde{x}^3 = ct - z$$

The point form

$$\tilde{x}^0 = \tau \quad , \quad ct = \tau \cosh\omega$$
$$\tilde{x}^1 = \omega \quad , \quad x = \tau \sinh\omega \sin\theta \cos\phi$$
$$\tilde{x}^2 = \theta \quad , \quad y = \tau \sinh\omega \sin\theta \sin\phi$$
$$\tilde{x}^3 = \phi \quad , \quad x = \tau \sinh\omega \cos\theta$$

Reproduced from: Quantum chromodynamics and other field theories on the light cone, Stanley J. Brodsky, Hans-Christian Pauli, Stephen S. Pinsky, Physics Reports, Volume 301, Issues 4-6, 1 August 1998, Pages 299-486

Lorentz transformations in the light-front

Lorentz transformations leave $x^2 - c^2t^2$ invariant.

Light front position: $x_- = x - ct$

Light front time: $x_+ = x + ct$

$$x^2 - c^2t^2 = (x + ct)(x - ct) = x_+ x_-$$

Lorentz transformations are diagonal in light-front

$$x_\pm \longrightarrow x_\pm \sqrt{\frac{1 \pm v\,/\,c}{1 \mp v\,/\,c}}$$

Start with a simple model

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{1}{2}m_B^2\phi^2 + i\bar{\psi}\gamma^\mu\partial_\mu\psi - m_F\bar{\psi}\psi - \lambda\phi\bar{\psi}\psi$$

1+1D - Total Energy E, Charge Q and momentum P are conserved.

In instant form quantization Fock space has particles of positive and negative momenta for given conserved total momenta.

$$\left|F;\bar{F};\tilde{B}\right\rangle = \left|{n_1}^{m_1},{n_2}^{m_2},\ldots,{n_N}^{m_N};{\bar{n}_1}^{\bar{m}_1},{\bar{n}_2}^{\bar{m}_2},\ldots,{\bar{n}_N}^{\bar{m}_N};{\tilde{n}_1}^{\tilde{m}_1},{\tilde{n}_2}^{\tilde{m}_2},\ldots,{\tilde{n}_N}^{\tilde{m}_\Lambda}\right\rangle$$

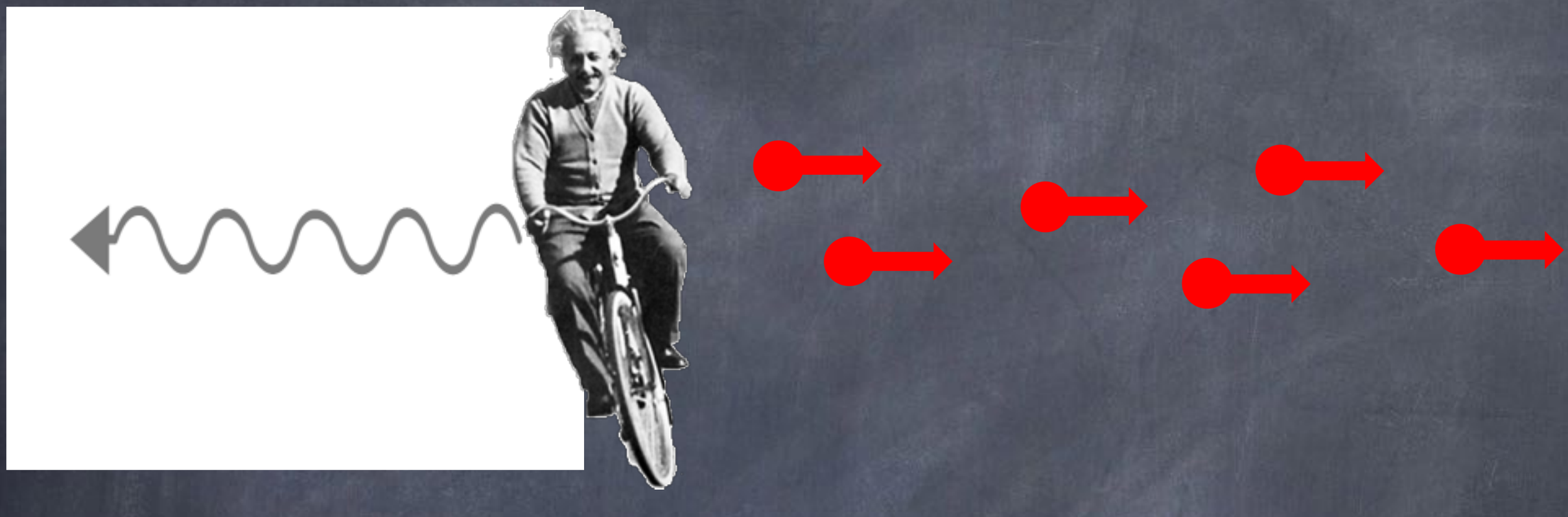
$$n_j,\bar{n}_j,\tilde{n}_j = 0,\pm1,\pm2,\pm3,\ldots,\pm\Lambda$$

This means cutoff introduces error in Hamiltonian.

This implies a large cutoff required to make this error small enough.

PRC 28 1679 (1983, Z. Phys. C 23 263 (1984), PRD, 32:1993-2000, (1985), PRD, 32(8):2001-2013, (1985).

Light-Front quantization in 1+1D



Think of an observer with x^- =const. - moving at c to the left.

This observer sees all massive particles moving to the right.

All massive particles have positive light front momentum.

Fock space is partitioned into sectors of total LF momentum

Start with a simple model in 1+1D

$$\mathcal{L} = \frac{1}{2}(\partial\phi)^2 - \frac{1}{2}m_B^2\phi^2 + i\bar{\psi}\gamma^\mu\partial_\mu\psi - m_F\bar{\psi}\psi - \lambda\phi\bar{\psi}\psi$$

Free Boson | Dirac Fermion | Interaction

Harmonic Resolution K: dimensionless light-front momentum

$$K = \sum_n n(a_n^\dagger a_n + b_n^\dagger b_n + d_n^\dagger d_n)$$

This plays the same role as electron number in chemistry

Charge:

$$Q = \sum_n (b_n^\dagger b_n - d_n^\dagger d_n)$$

PRC 28 1679 (1983, Z. Phys. C 23 263 (1984), PRD, 32:1993-2000, (1985), PRD, 32(8):2001-2013, (1985).

Light-Front Fock space in 1+1 D

Light-front quantization gives Fock space states:

$$\left|F;\bar{F};\tilde{B}\right\rangle = \left|1^{m_1},2^{m_2},...,\Lambda^{m_\Lambda};\bar{1}^{\bar{m}_1},\bar{2}^{\bar{m}_2},...,\Lambda^{\bar{m}_\Lambda};\tilde{1}^{\tilde{m}_1},\tilde{2}^{\tilde{m}_2},...,\Lambda^{\tilde{m}_\Lambda}\right\rangle$$

$$m_i,\bar{m}_i \in \{0,1\} \qquad 0 \le \tilde{m}_i < \Lambda \,/\, i+1$$

Total Light-front momenta is partitioned amongst the particles

Light-front momentum and energy depend simply on L:

Momentum $P^+ = \frac{2\pi}{L}K$ $\qquad$ $P^- = \frac{L}{2\pi}H$ Energy

Different values of K label blocks of the light-front Hamiltonian

Harmonic resolution K is a good quantum number instead of particle number.

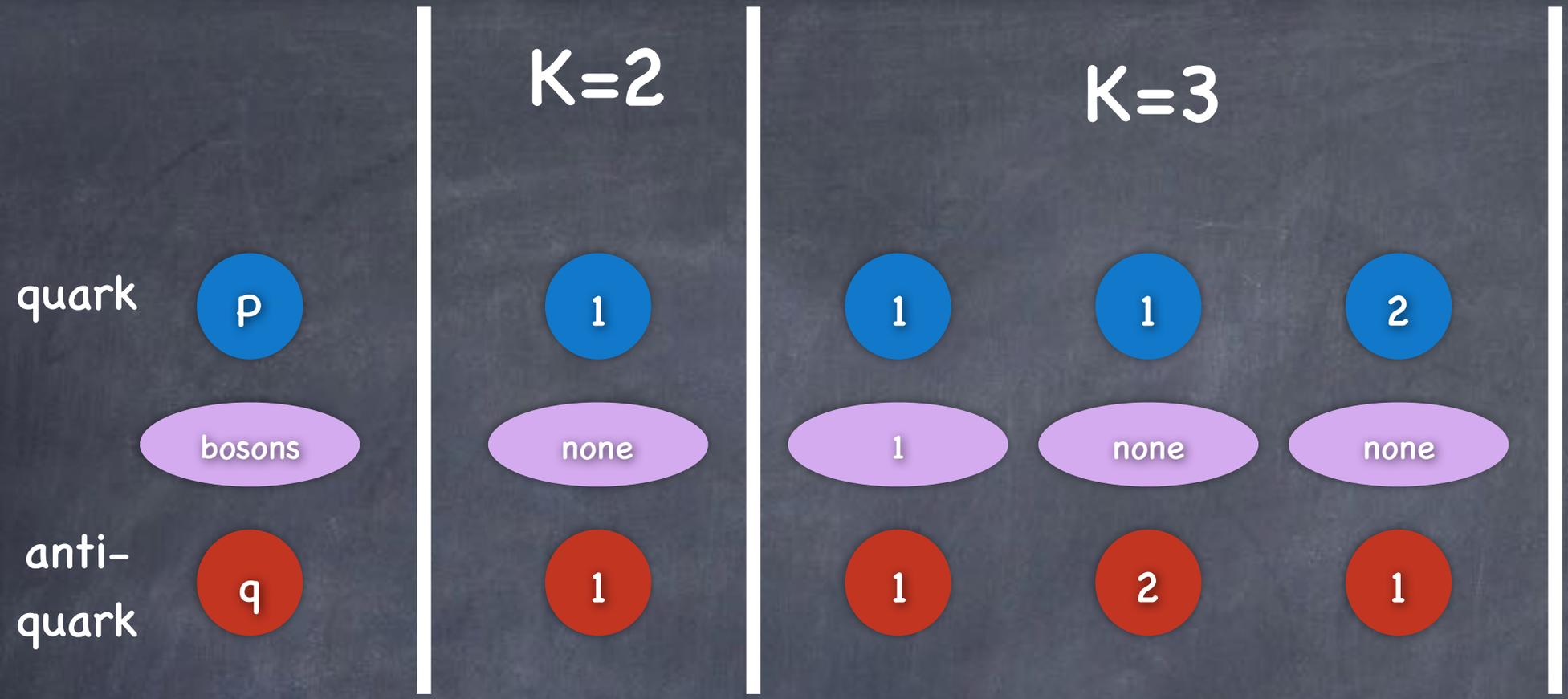
What is the meaning of Harmonic Resolution?

Compton wavelength of mass m particle: wavelength of photon with energy mc^2

$$\lambda_C = \frac{h}{mc}$$

Harmonic resolution is ratio of box size to Compton wavelength: K is a "resolving power"

$$K = \frac{L}{\lambda_C}$$

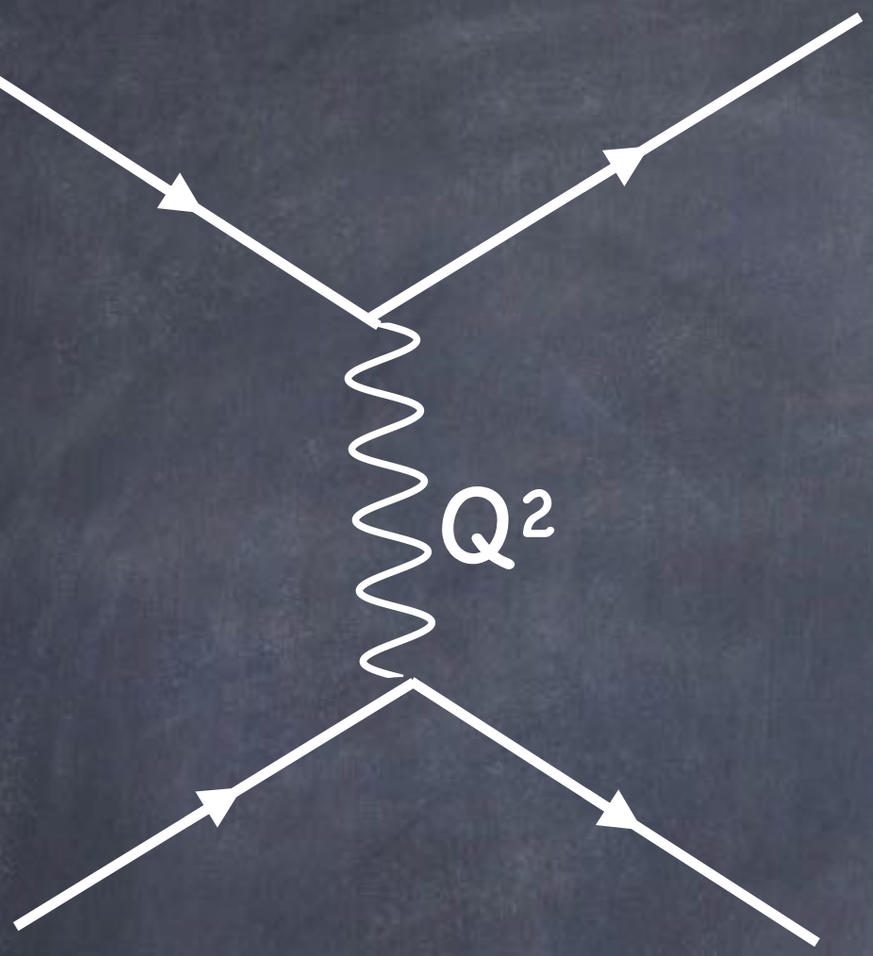


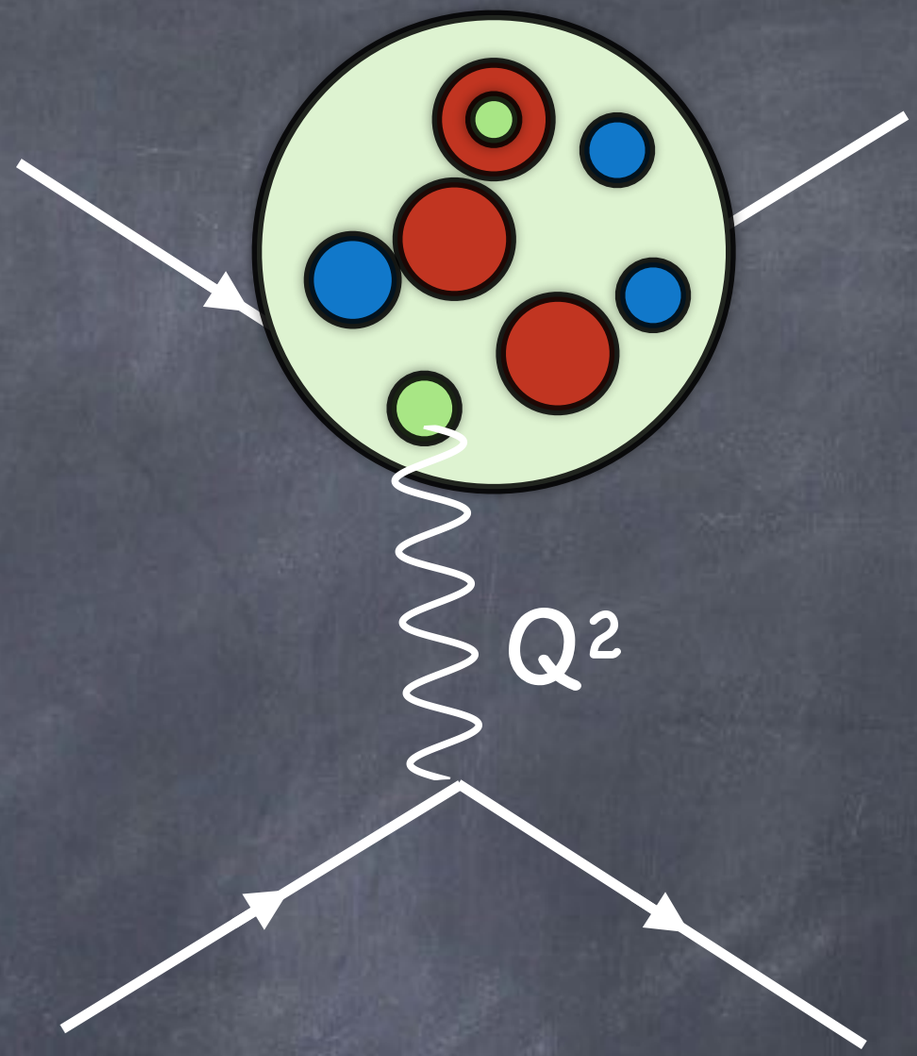
Interacting theory has bound states of constituents whose properties emerge from the theory

Example: mesons - fermion-antifermion pairs with different momenta and numbers of binding bosons.

Structure of these particles is encoded in PDF

What do we want to compute?





What is the probability that a given constituent carries a fraction of the light front momentum x?

$$x = \frac{p^+}{P^+} \qquad 0 \leq x \leq 1$$

Parton Distribution Function

What is the probability that a given constituent carries a fraction of the light front momentum x?

$$x = \frac{p^+}{P^+} \qquad 0 \leq x \leq 1$$

Harmonic Resolution K gives a PDF with K points:

$$f(x) = f\left(\frac{p^+}{P^+}\right) = f\left(\frac{n}{K}\right) = \sum_i \widehat{m}_i^{(n)} \left|\langle \phi_i^{(n)} | \Psi_K \rangle\right|^2 \quad .$$

All fock states with constituents carrying n quanta of harmonic resolution K. This is the expectation value of a one-body operator in the front form.

Compact Mapping to Qubits in 1+1D

$$\left|F;\bar{F};\tilde{B}\right\rangle = \left|1^{m_1},2^{m_2},...,\Lambda^{m_\Lambda};\bar{1}^{\bar{m}_1},\bar{2}^{\bar{m}_2},...,\Lambda^{\bar{m}_\Lambda};\tilde{1}^{\tilde{m}_1},\tilde{2}^{\tilde{m}_2},...,\Lambda^{\tilde{m}_\Lambda}\right\rangle$$

$$m_i,\bar{m}_i \in \{0,1\} \qquad 0 \le \tilde{m}_i < \Lambda / i+1$$

Only store occupied orbitals. Worst case state is:

$$\left|1^1 2^1 3^1 4^1 ... I^1\right\rangle \qquad K = \sum_{l=1}^{I} l = \frac{I(I+1)}{2}$$

Number of occupied orbitals I scales as $\sqrt{K}$

Requires $\tilde{O}\left(\sqrt{K}\right)$ qubits in 1+1D

Simulation cost in 1+1D

Quantum simulation algorithms now depend optimally on:

1. Sparsity -$O(K^2)$
2. Norm (can use max norm - largest matrix element O(K))
3. Cost of locating and computing matrix elements - O(K).
4. Inverse error - logarithmic.

Overall cost of simulation for time t is $\tilde{O}\left(tK^4\right)$

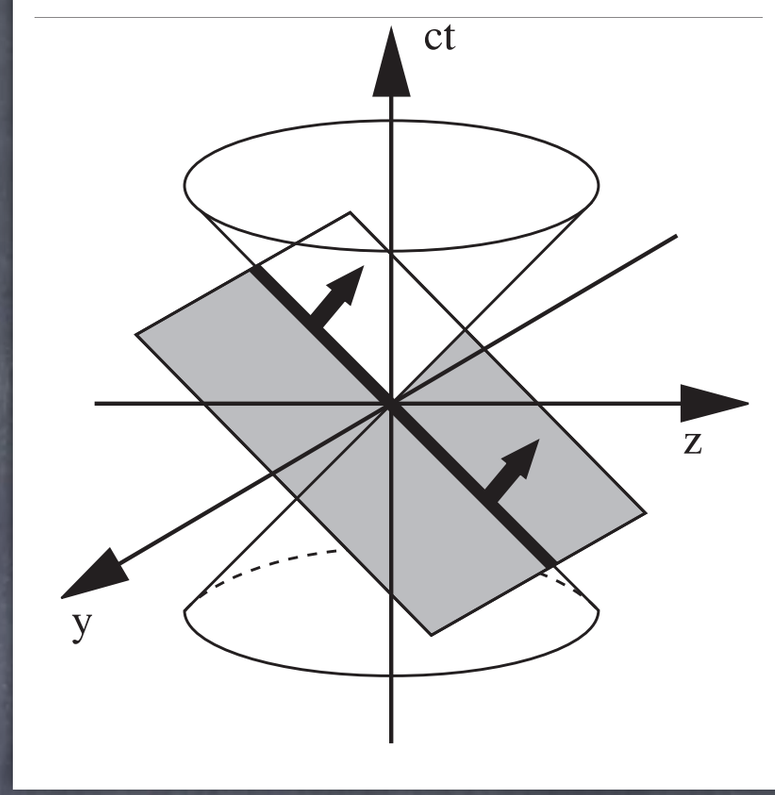
Adiabatic state preparation costs $\tilde{O}\left(TK^4\right)$

D. W. Berry, A. M. Childs, and R. Kothari, "Hamiltonian simulation with nearly optimal dependence on all parameters", in: 2015 IEEE 56th Annual Symposium on Foundations of Computer Science, IEEE, 2015, pp. 792–809.
D. W. Berry, A. M. Childs, Y. Su, X. Wang, and N. Wiebe, "Time-dependent Hamiltonian simulation with L1-norm scaling", arXiv: 1906.07115, 2019.

Compact Mapping to Qubits in 3+1D

Transverse momenta mean multiple orbitals with same light front momenta, but distinct other quantum numbers.

$$\left|\left\{\{K_i, k_i^1, k_i^2\}\,|\,1 \le i \le I\right\}\right\rangle$$



Worst case state is when all occupied modes have light-front momentum 1

$$\left|\left\{\{1_i, k_i^1, k_i^2\}\,|\,1 \le i \le K\right\}\right\rangle = \left|\left\{1, k_1^1, k_1^2\right\}, \left\{1, k_2^1, k_2^2\right\} .. \left\{1, k_K^1, k_K^2\right\}\right\rangle$$

Qubit requirements scale as $O\Big(K\Big(\log \Lambda_\perp + \log K\Big)\Big)$

Counting qubits for 3+1D QCD

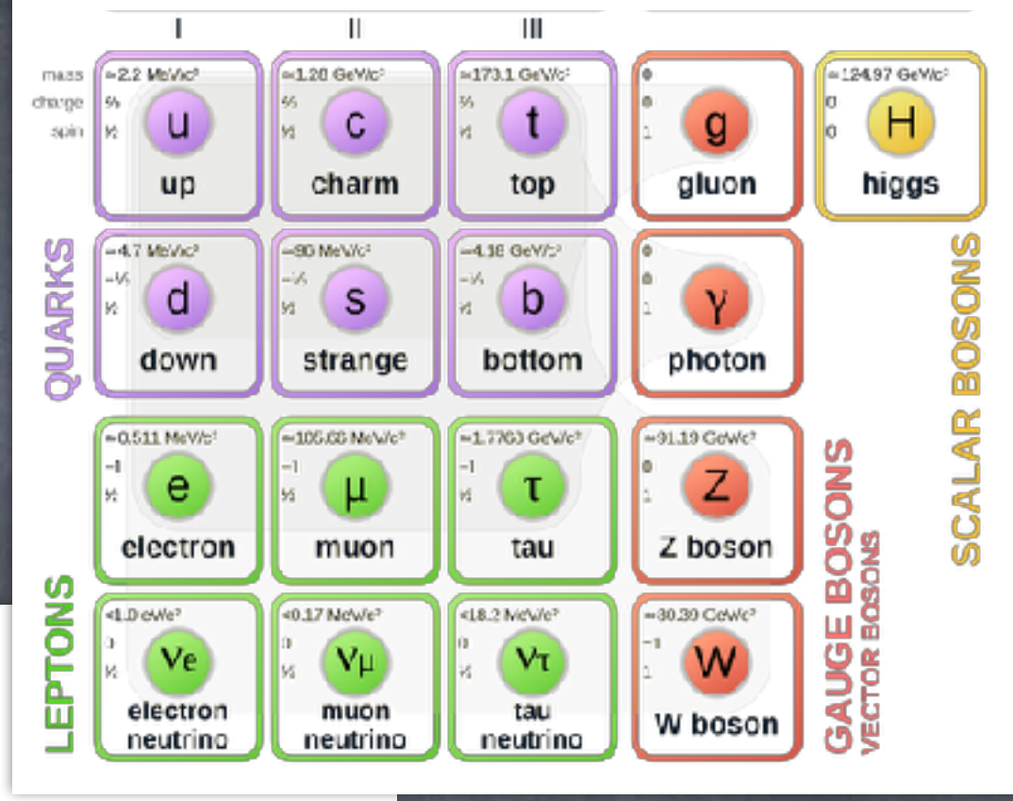
Lattice approaches daunting:

20^3 grid for 3+1 QCD:

400000 qubits.

$$\mathrm{Q} \leq \underbrace{2K}_{\substack{\text{number of}\\ \text{occupied}\\ \text{fermion/antifermion}\\ \text{modes}}} \Big[\underbrace{\underbrace{\lceil \log_2 K \rceil}_{\text{momentum}} + 2\lceil \log_2 \Lambda_\perp \rceil}_{\text{fermion/antifermion mode quantum numbers}} + \underbrace{1}_{\text{helicity}} + \underbrace{\lceil \log_2 n_f \rceil}_{\text{flavors}} + \underbrace{\lceil \log_2 n_c \rceil}_{\text{colors}} \Big]$$

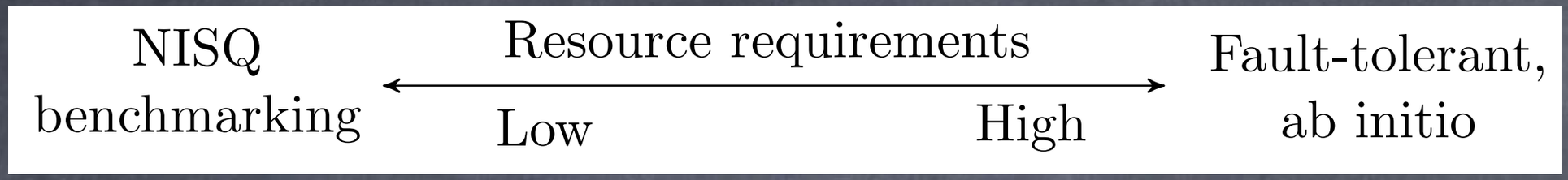
$$+ \underbrace{K}_{\substack{\text{number of}\\ \text{occupied}\\ \text{boson modes}}} \Big[\underbrace{\underbrace{\lceil \log_2 K \rceil}_{\text{momentum}} + 2\lceil \log_2 \Lambda_\perp \rceil}_{\text{boson mode quantum numbers}} + \underbrace{\lceil \log_2 K \rceil}_{\text{occupancy}} + \underbrace{1}_{\text{helicity}} + \underbrace{\lceil \log_2 (n_c^2 - 1) \rceil}_{\text{colors}} \Big]$$



For 20^3 grid for 3+1 QCD Q=1360 qubits

This is smaller than 400000

Light-Front simulations on NISQ devices



Can we do some calculations on existing devices?

Basis Light Front Quantization: effective light-front Hamiltonian + second quantization + smart basis choice

Very efficient representations of QFT.

Example: light mesons.

BLFQ in 3 + 1D (arXiv:2009.07885.)

1. Restrict to valence sector of meson Fock space
2. Work in terms of relative momentum: as for Hydrogen atom in basic QM.
3. Use an effective Hamiltonian (1811.08512)

$$H = H_0 + H_{NJL,\pi} = H_{\text{transverse}} + H_{\text{longitudinal}} + H_{NJL,\pi}$$

4. H_0 can be solved analytically and its eigenstates provide an efficient basis representation for the problem
5. H_{NJL} is the Nambu-Jona-Lasinio (two people!) interaction - an effective four fermion interaction.

S. Klimt, M. F. M. Lutz, U. Vogl, and W. Weise, Nucl. Phys. A516, 429 (1990).

S. P. Klevansky, Rev. Mod. Phys. 64, 649 (1992)

Shaoyang Jia and James P. Vary Phys. Rev. C 99, 035206 (2019)

BLFQ in 3 + 1D (arXiv:2009.07885.)

Just as in chemistry we can specify the absolutely minimal model - analogous to STO3G H2.

$$h_{ij} = \begin{pmatrix} 640323 & 139872 & -139872 & -107450 \\ 139872 & 346707 & 174794 & 139872 \\ -139872 & 174794 & 346707 & -139872 \\ -107450 & 139872 & -139872 & 640323 \end{pmatrix}$$

Eigenvalues $\{139.6^2, 722.2^2, 827.8^2, 864.7^2\}$ MeV^2

Two lowest eigenvalues should be compared with masses of Pi$^+$ and rho$^+$ mesons $\{139.57^2, 775.26^2\}$ MeV^2

Simplest testbed problem.

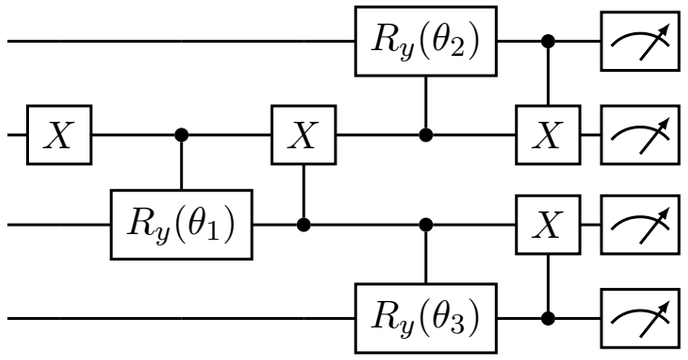
S. Klimt, M. F. M. Lutz, U. Vogl, and W. Weise, Nucl. Phys. A516, 429 (1990).

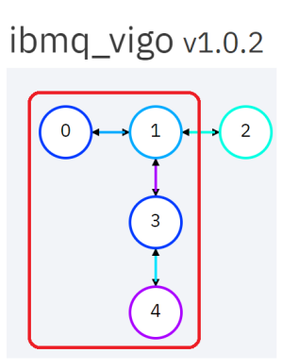
S. P. Klevansky, Rev. Mod. Phys. 64, 649 (1992)

Shaoyang Jia and James P. Vary Phys. Rev. C 99, 035206 (2019)

BLFQ in 3 + 1D (arXiv:2009.07885.)

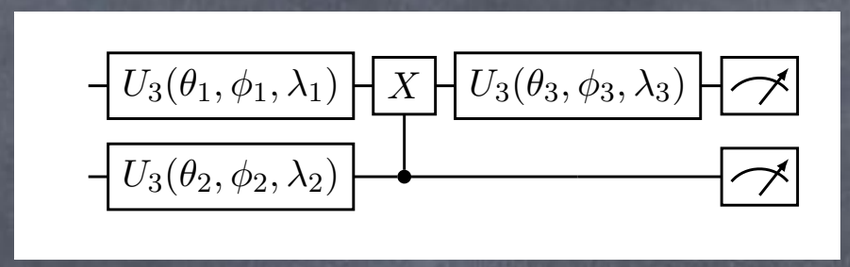
Direct Mapping





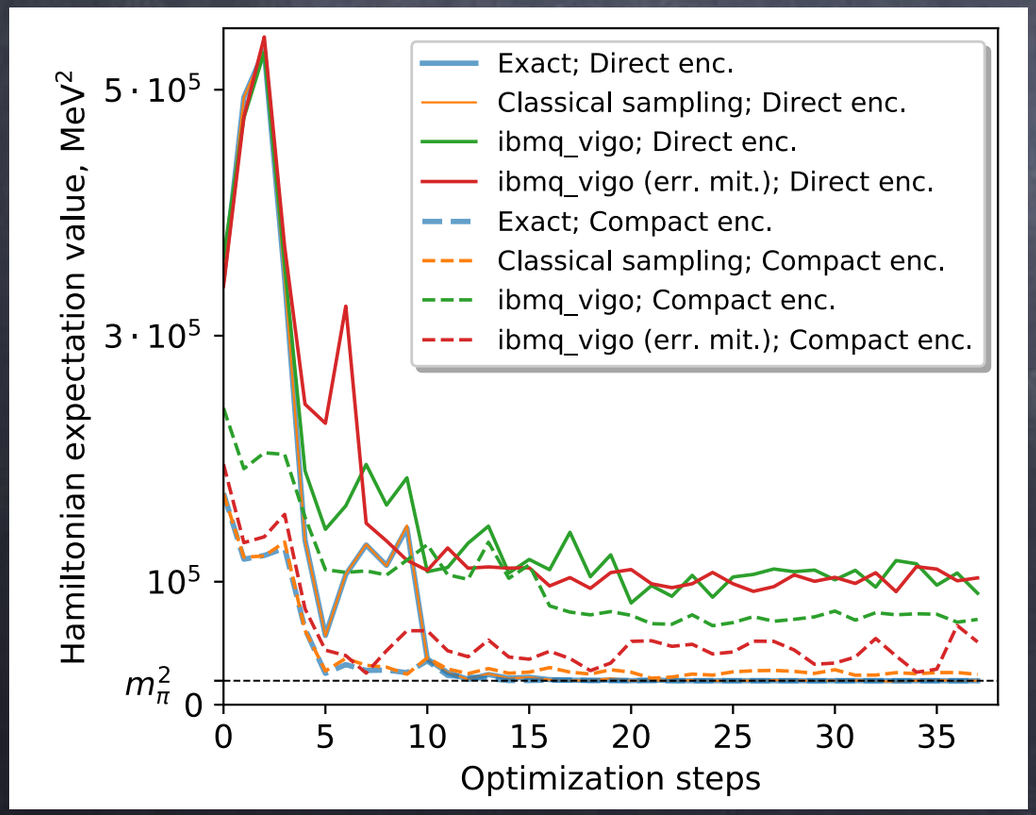
Four qubits, sixteen Pauli terms

Compact Mapping



Two qubits, five Pauli terms

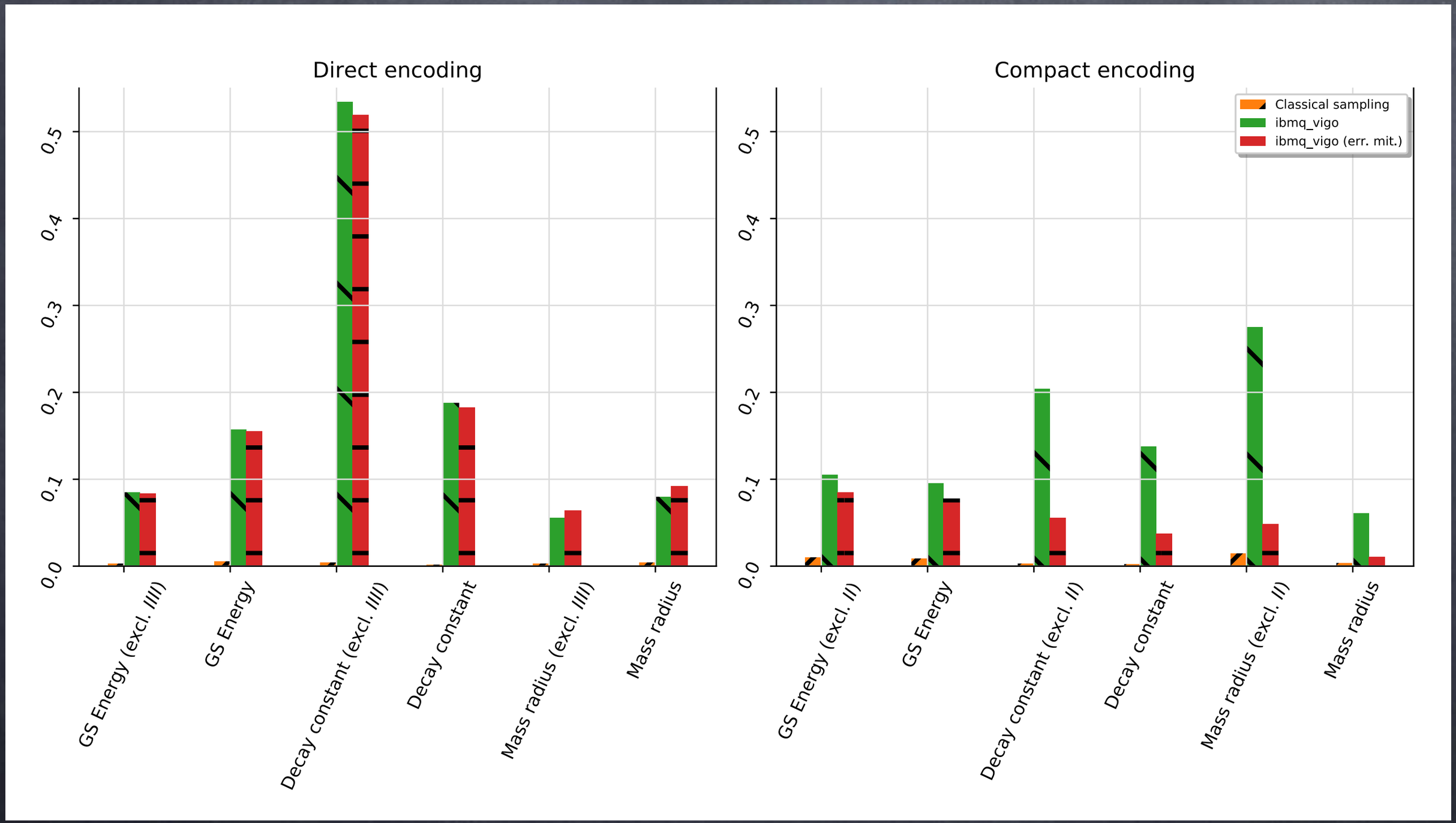
IBM vigo, 8192 samples per term



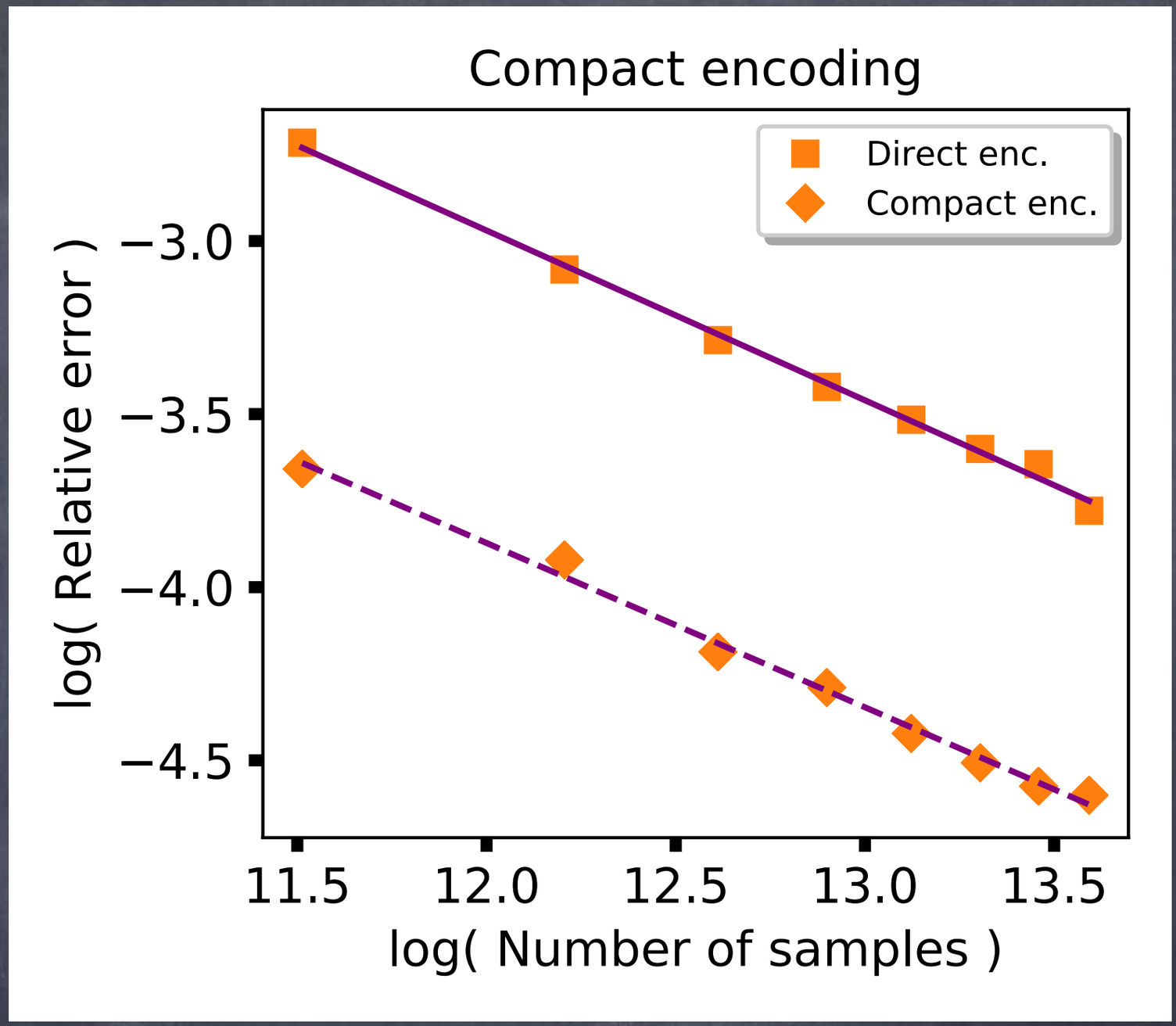
Here we optimize the ansatz by minimizing particle mass.

Given the optimized ansatz, we can compute other particle properties by estimating other observables.

BLFQ in 3 + 1D (arXiv:2009.07885.)



Errors: mass



Precision vs. number of samples for ground state energy obtained via sampling from the exact distribution. Fitting gives $n \approx 382/\varepsilon^{2.04}$ (direct encoding) and $n \approx 46/\varepsilon^{2.1}$ in (compact encoding), confirming the theoretical $n \sim O(1/\varepsilon^2)$ dependence. (Natural logs).

Errors: charge radius

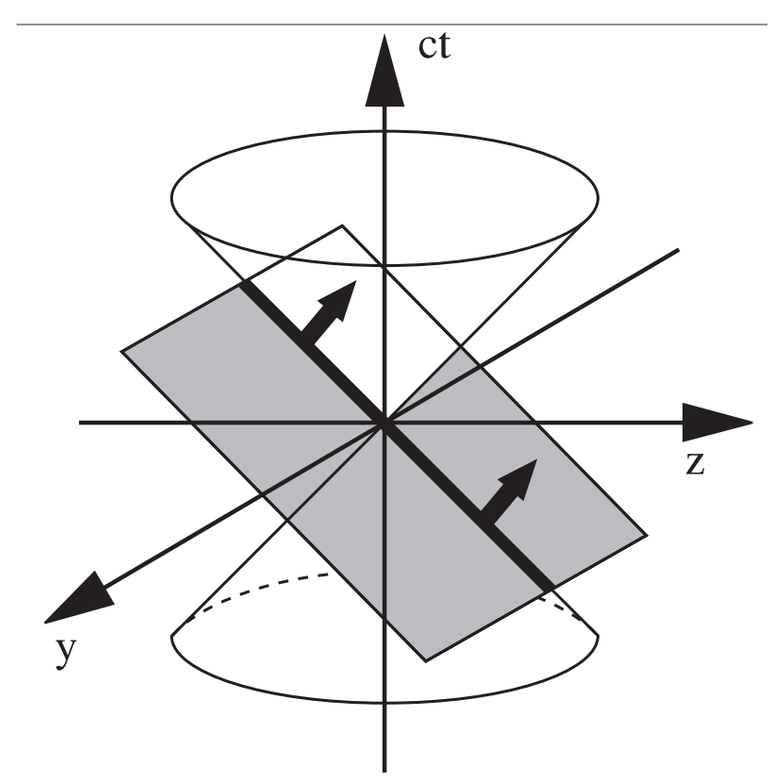
	Charge radius $\sqrt{\langle r_c^2 \rangle}$, $\mathbf{MeV}^{-1}$	
Encoding	Direct	Compact
Exact	$6.31 \cdot 10^{-3}$	$6.31 \cdot 10^{-3}$
Classical sampling	$6.29 \cdot 10^{-3}$	$6.30 \cdot 10^{-3}$
`ibmq_vigo`	$6.33 \cdot 10^{-3}$	$6.35 \cdot 10^{-3}$
`ibmq_vigo` (err. mit.)	$6.34 \cdot 10^{-3}$	$6.31 \cdot 10^{-3}$

Summary

VQE [2, 3] | Fault-tolerant [1]

Two-body sector BLFQ, relative coordinate basis	→	Valence sector BLFQ, single-particle basis	→	Multi-particle BLFQ, single-particle basis	→	Multi-particle DLCQ single-particle basis

Benchmarking | Quantum-computational advantage



[1] Quantum Simulation of Quantum Field Theory in the Light-Front Formulation, arXiv:2002.04016

[2] Light-Front Field Theory on Current Quantum Computers, arXiv:2009.07885.

[3] Simulating High Energy Physics on NISQ devices using Basis Light-Front Quantization (in preparation).

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