

Quantum Simulation of Nuclear Effective Field Theories

(Manuscript in Progress)

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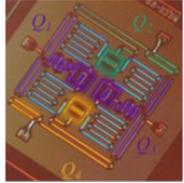
Alexey Gorshkov



Alex Shaw

- Overview of Chiral Effective Field Theory
- Quantum Simulation
- Optimising Quantum Simulation of Chiral Effective Field Theories for Digital Quantum Computers
- Cost Estimates for Nuclear Spectroscopy

UMD's ion trap quantum chip, Image by E. Edwards



IBM superconductor quantum chip, Córcoles et al.

Quantum simulation and quantum computation?

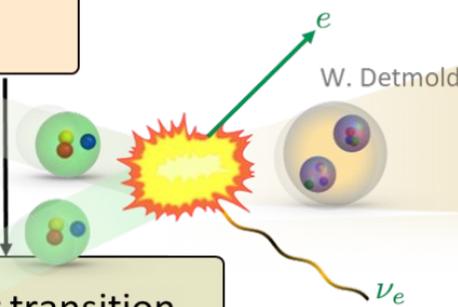
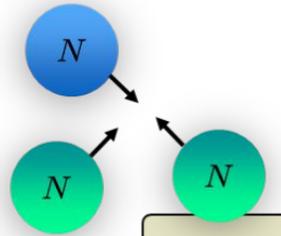
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Dana Berry, Skyworks Digital, Inc.



Standard Model (QCD)



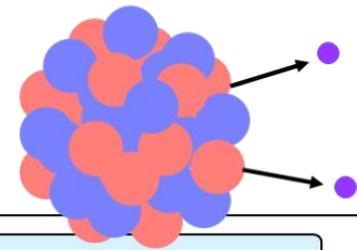
Nuclear and hypernuclear interactions

Nuclear transition amplitudes

Effective field theory of forces

Effective field theory of nuclear responses to external probes

Many-body structure and dynamics calculations



Supernovae and origin of heavy elements

Exotic phases of strongly interacting matter

Violation of symmetries in nuclei and hidden new interactions in nature

Neutron star equation of state and their mergers

How finely tuned is the carbon-based life on earth?

Nature of dark matter and its interactions with ordinary matter

Theory

Few-body physics

Many-body physics

Diagram: Zohreh Davoudi

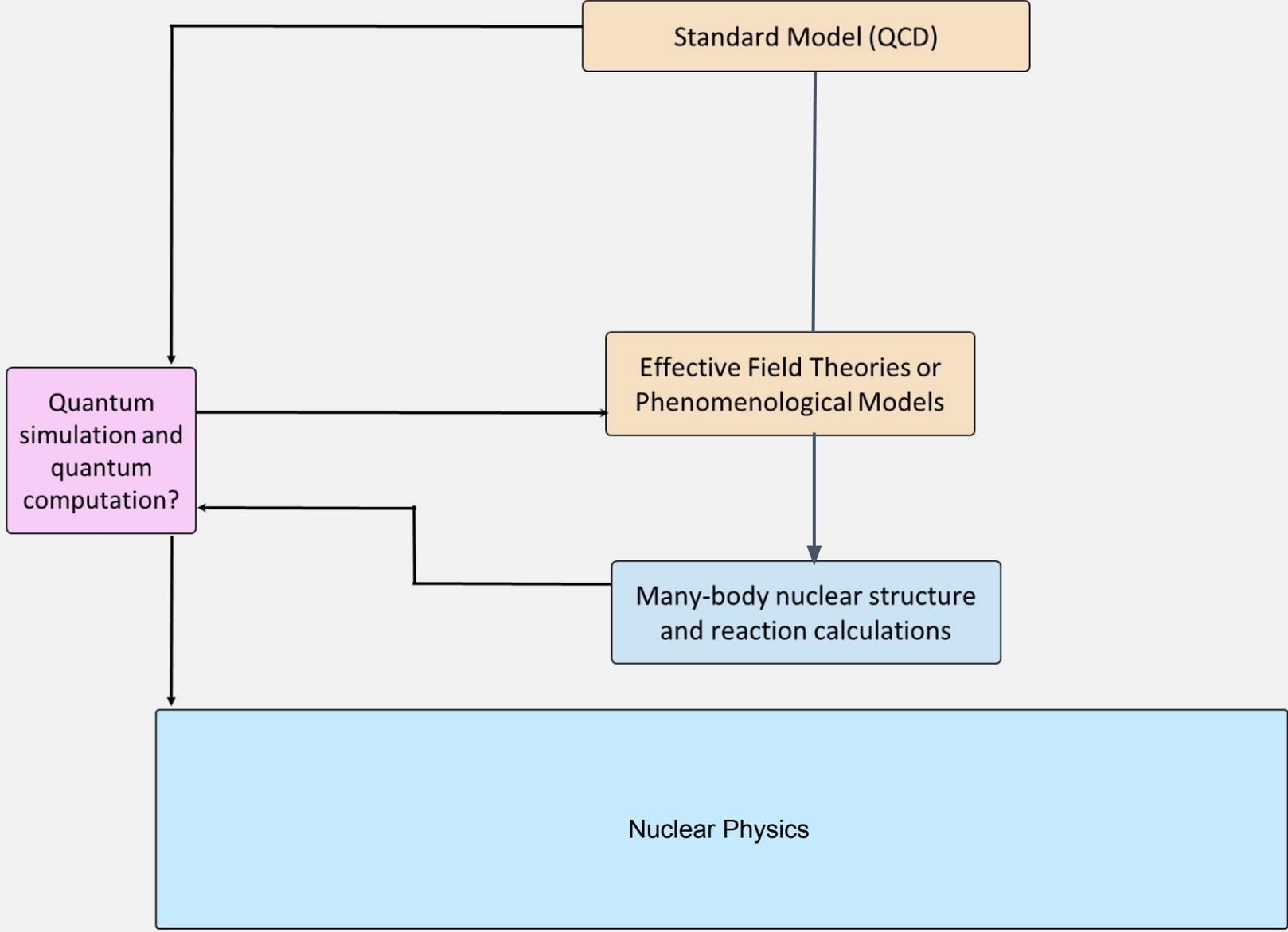


Diagram:
Zohreh Davoudi

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 - Scattering cross-sections
 - Low-lying spectra
 - etc.

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- Could try QCD from first principles:
 - Classical MC can currently just simulate deuterium.
 - Quantumly, first estimates of simple quark transport properties need $>10^{50}$ gates¹.
- Semi-empirical models (e.g. mean field) aren't reliable for large nuclei or theoretically well justified.

Approaching Nuclear Physics with EFTs: Chiral EFT



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- Treats protons, neutrons and pions as the degrees of freedom of the theory.
- Nucleons described by non-relativistic dynamics.

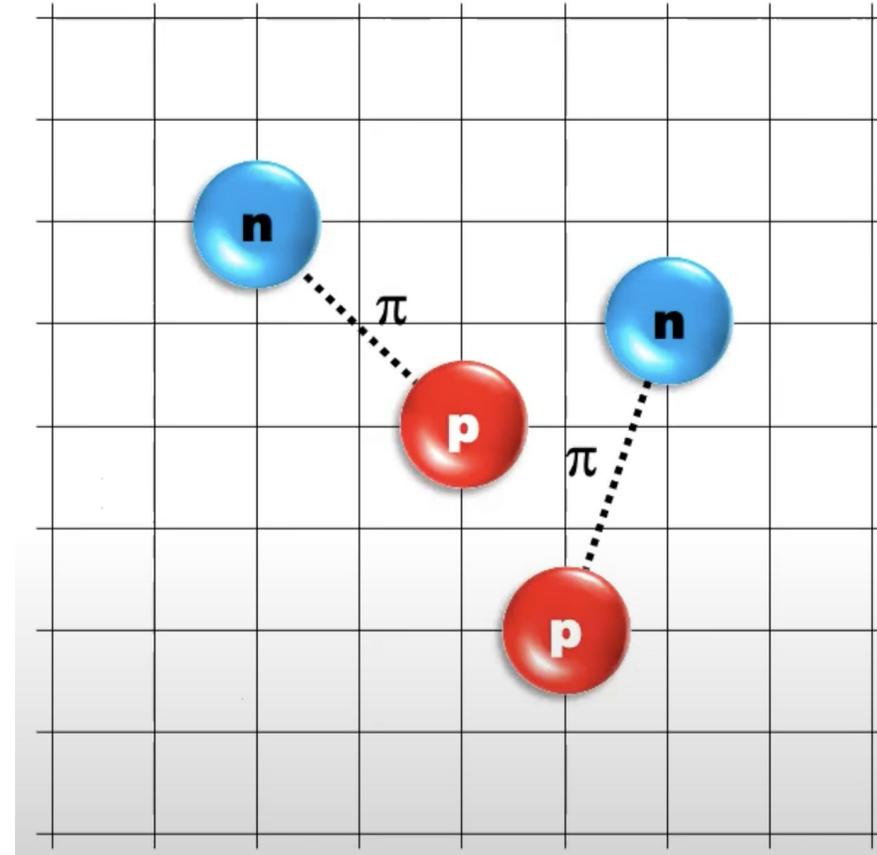


Image: Dean Lee

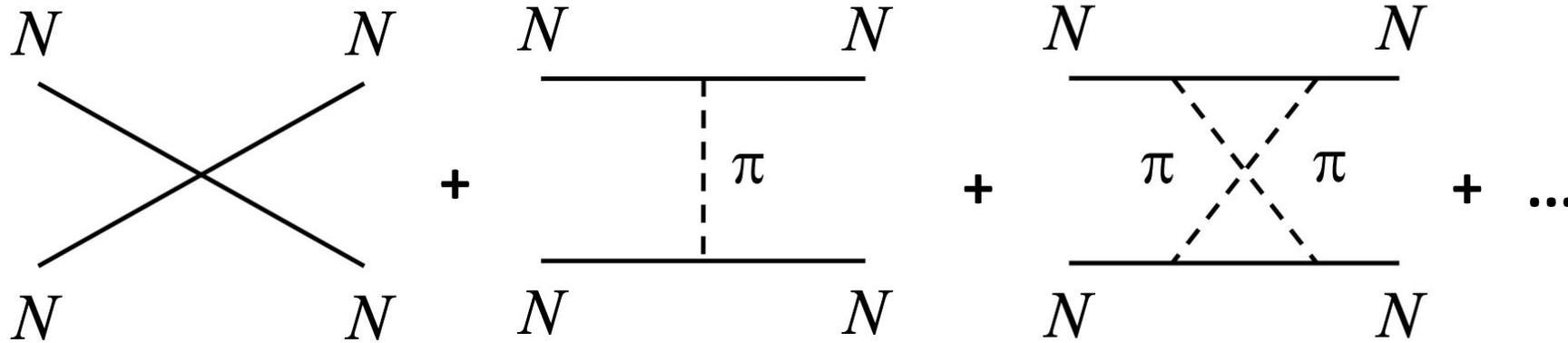
To leading order the Lagrangian looks something like this:

$$\begin{aligned}
 \hat{\mathcal{L}}^{\Delta=0} = & \frac{1}{2} \partial_\mu \boldsymbol{\pi} \cdot \partial^\mu \boldsymbol{\pi} - \frac{1}{2} m_\pi^2 \boldsymbol{\pi}^2 \\
 & + \frac{1-4\alpha}{2f_\pi^2} (\boldsymbol{\pi} \cdot \partial_\mu \boldsymbol{\pi})(\boldsymbol{\pi} \cdot \partial^\mu \boldsymbol{\pi}) - \frac{\alpha}{f_\pi^2} \boldsymbol{\pi}^2 \partial_\mu \boldsymbol{\pi} \cdot \partial^\mu \boldsymbol{\pi} + \frac{8\alpha-1}{8f_\pi^2} m_\pi^2 \boldsymbol{\pi}^4 \\
 & + \bar{N} \left[i\partial_0 - \frac{g_A}{2f_\pi} \boldsymbol{\tau} \cdot (\vec{\sigma} \cdot \vec{\nabla}) \boldsymbol{\pi} - \frac{1}{4f_\pi^2} \boldsymbol{\tau} \cdot (\boldsymbol{\pi} \times \partial_0 \boldsymbol{\pi}) \right] N \\
 & + \bar{N} \left\{ \frac{g_A(4\alpha-1)}{4f_\pi^3} (\boldsymbol{\tau} \cdot \boldsymbol{\pi}) \left[\boldsymbol{\pi} \cdot (\vec{\sigma} \cdot \vec{\nabla}) \boldsymbol{\pi} \right] + \frac{g_A \alpha}{2f_\pi^3} \boldsymbol{\pi}^2 \left[\boldsymbol{\tau} \cdot (\vec{\sigma} \cdot \vec{\nabla}) \boldsymbol{\pi} \right] \right\} N \\
 & - \frac{1}{2} C_S \bar{N} N \bar{N} N - \frac{1}{2} C_T (\bar{N} \vec{\sigma} N) \cdot (\bar{N} \vec{\sigma} N) + \dots,
 \end{aligned}$$

Modelling Nuclear Physics: Chiral EFT



The physical model you should have in your head is:



Contact Interactions

Single Pion Exchange

Two Pion Exchange

Higher order terms are more relevant at higher momenta



Simulating Chiral EFTs



Classically simulate time evolution:

=> sign problem!

=> huge resource costs

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Quantumly simulate time evolution:

=> provably no sign problem!

=> “efficient”

How feasible is quantum simulation of Chiral EFT?

Our Work



Our Work

- We determine gate counts for NISQ and fault-tolerant quantum computers for time evolution and spectroscopy of nuclei.
- For 4 different Hamiltonians corresponding to the leading order terms in the Effective Field Theory expansion.
- Improve on fermionic encodings, bosonic encodings, error analysis, etc. to minimise gate counts and determine which is the most feasible.
- Allows us to compare efficiency of simulating leading order EFT Hamiltonians.



Time Evolution Algorithms

EFTs and Quantum Computing



- Time evolution is an important primitive, e.g. for quantum phase estimation.

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- Try simulating using product formulae. For Hamiltonian:

$$H = \sum_{\gamma=1}^{\Gamma} H_{\gamma}$$

$$e^{-iH\delta t} \approx e^{-iH_1\delta t} e^{-iH_2\delta t} \dots e^{-iH_{\Gamma}\delta t} =: \mathcal{P}(\delta t)$$

$$\|e^{-iH\delta t} - \mathcal{P}(\delta t)\| \leq \epsilon$$

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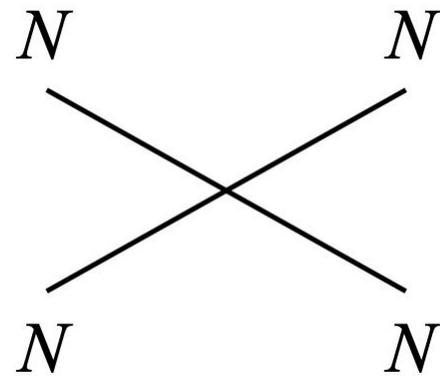
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- Product formulae have low overhead and generally perform well!
- *How well can we improve our error bounds and optimise computational resources when simulating Chiral Effective Field Theories?*

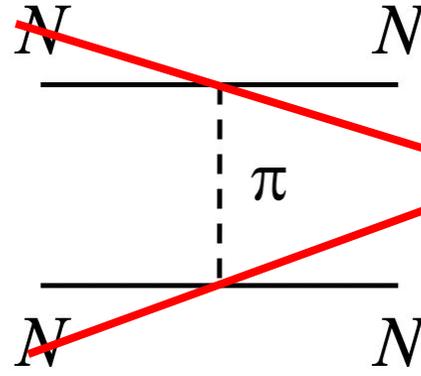
Optimising Simulation for the Simplest Theory: Pionless EFT

- Pionless EFT is the simplest Hamiltonian that recreates basic properties of the nucleus¹ for momenta below pion mass.



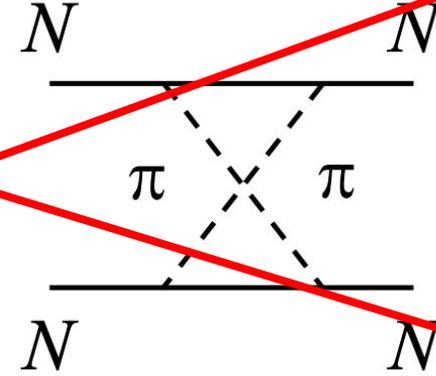
Contact Interactions

+



Single Pion Exchange

+



Two Pion Exchange

¹See works by: Kaplan, Savage, van Kolck, Bedaque...

- Pionless EFT is the simplest Hamiltonian that recreates basic properties of the nucleus¹.
- Discretise the theory and put on a 3D lattice rather continuous space:
- We choose a 2nd quantisation and position-space formulation.

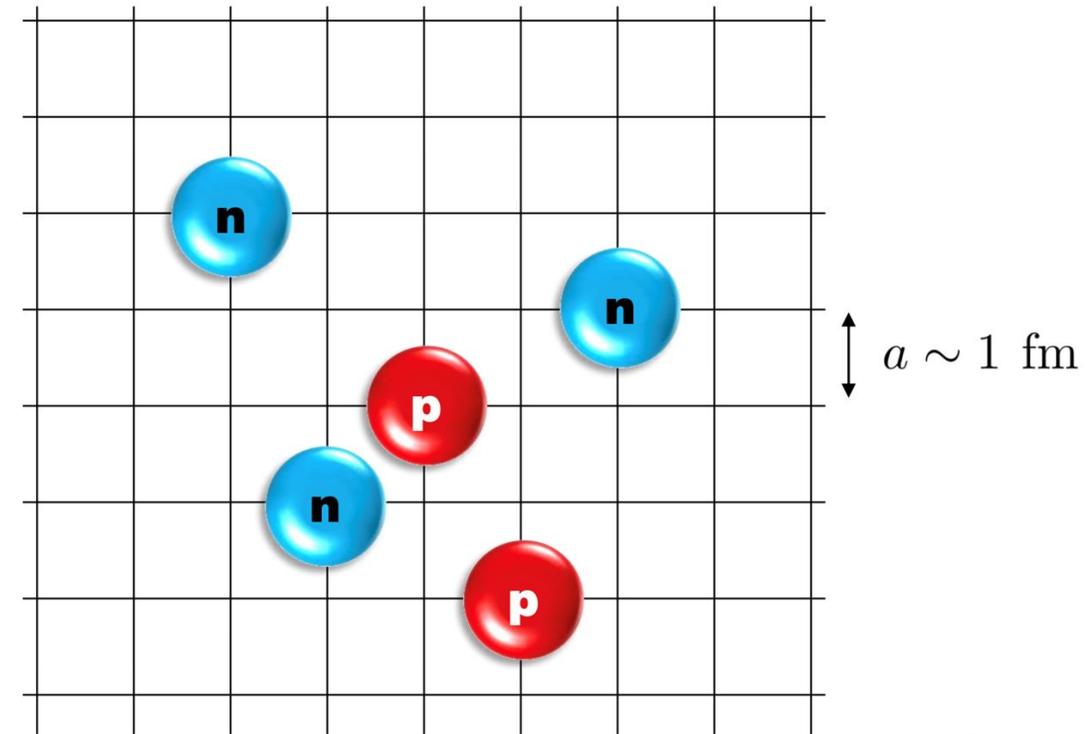


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Creation and annihilation operators for nucleons.

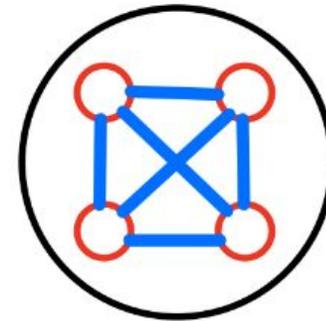
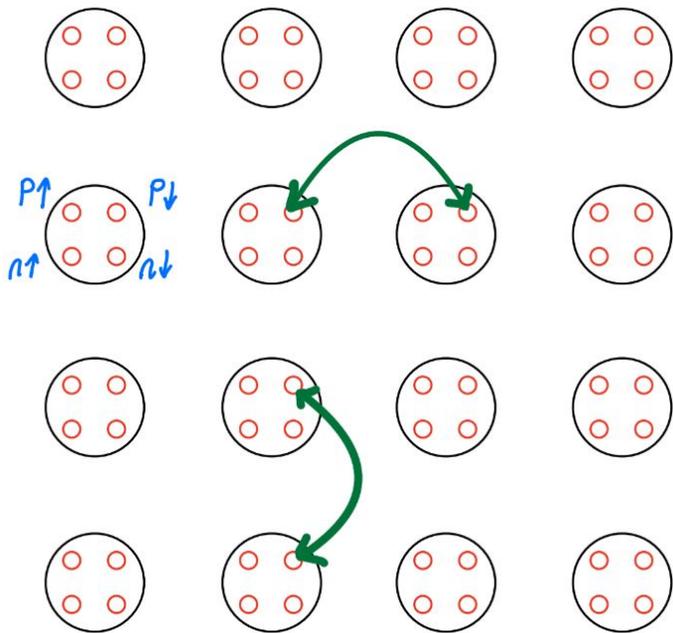
Nucleon number operator at site i .

$$\sigma \in \{p \uparrow, p \downarrow, n \uparrow, n \downarrow\}$$

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Take advantage of as many details as possible to reduce simulation costs!

¹See works by: Kaplan, Savage, van Kolck, Bedaque...

Fermionic Encodings



- In simulating the pionless EFT, the most expensive term is the kinetic hopping term.

Fermionic Encodings

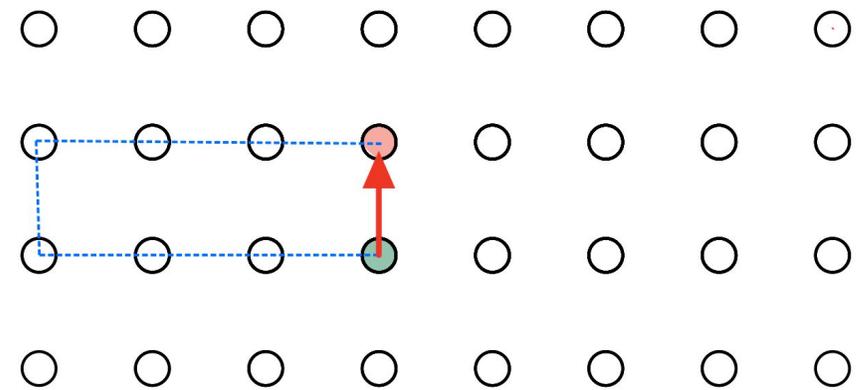
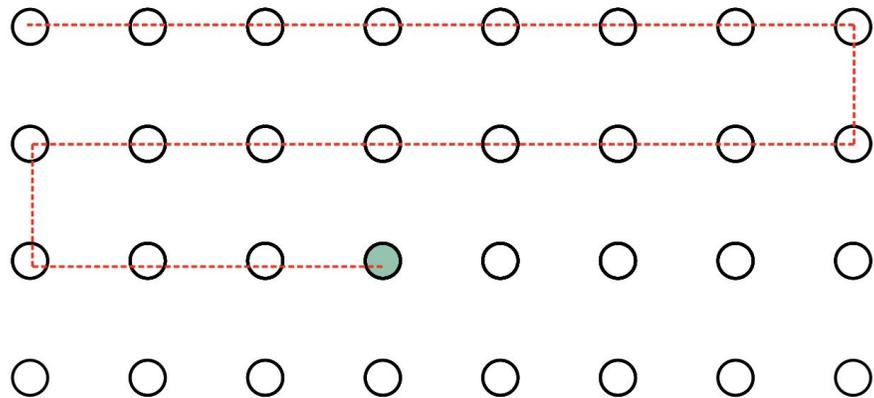


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- Due to non-locality of fermions:
 - If fermions are encoded via Jordan-Wigner mapping, this term takes $O(L^{D-1})$ gates to implement.
 - Alternatives: Fast Fermionic Fourier Transform/SWAP Network/Givens Rotation, need gate depth proportional to number of fermionic modes.

Fermionic Encodings



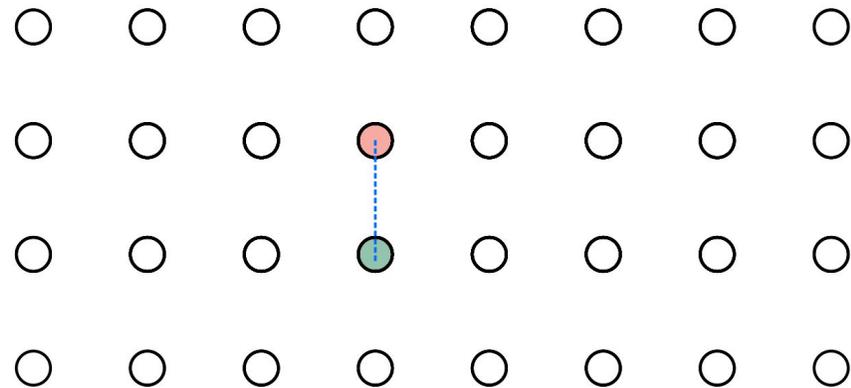
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 - Alternatives: Fast Fermionic Fourier Transform/SWAP Network/Givens Rotation, need gate depth proportional to number of fermionic modes.
- Leverage interaction locality + fermion no. conservation: encode fermions using Verstraete-Cirac or Compact encoding.
 - Implement a single hopping operator in $O(1)$ depth

Implementing each Trotter Step



- Fermionic encoding + Hamiltonian structure allows a highly parallelizable implementation of each Trotter step.
- Allows for each term to be implemented in $O(1)$ depth and the Trotter step to have $O(1)$ depth.

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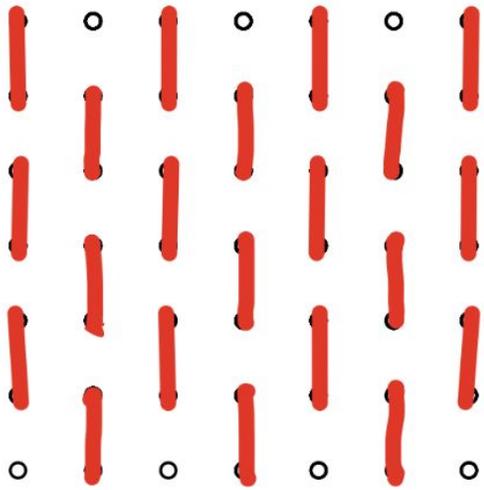
$$\overbrace{\sum_{\langle i,j \rangle} \left(a_{\sigma}^{\dagger}(i) a_{\sigma}(j) + a_{\sigma}^{\dagger}(j) a_{\sigma}(i) \right)}^{\text{kinetic term}}$$

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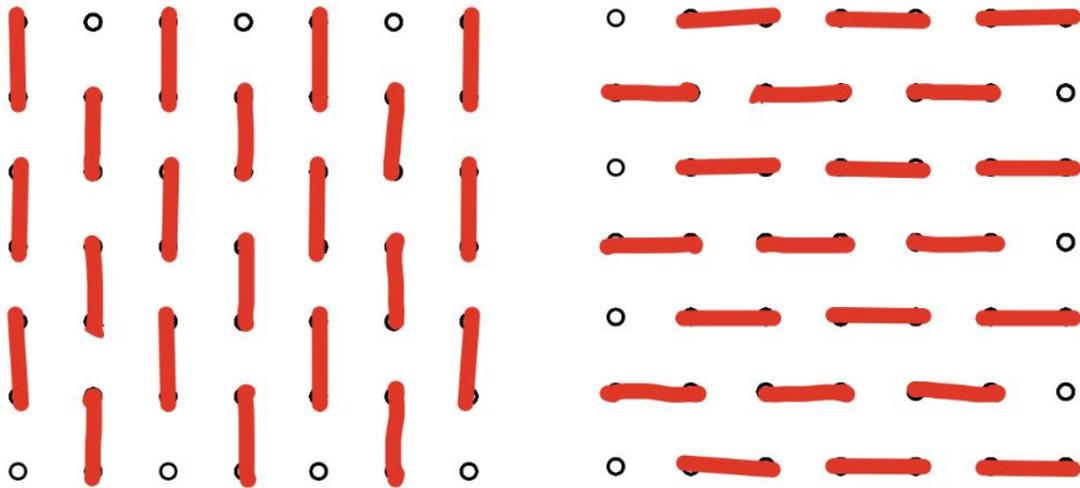
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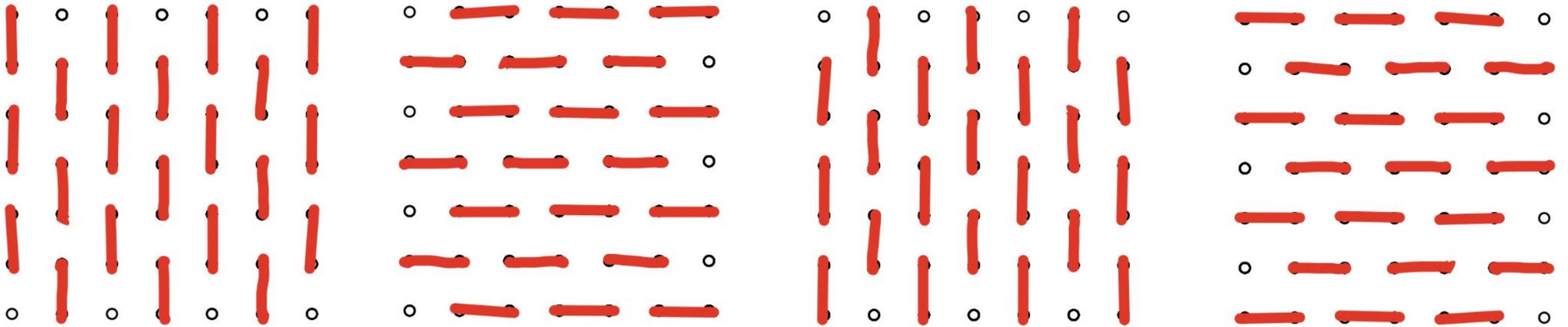
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Fermionic Encoding	Circuit Depth	Number of Qubits
Jordan-Wigner (Naive)	$O(M^2)$	M
FFFT/SWAP Networks	$O(M)$	M
VC or Compact	110	$1.5M$

($M = \#$ fermion modes, $M=4,000$ for $10 \times 10 \times 10$ lattice)

Fermionic Encodings



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- Hamiltonian is number preserving for each type of fermion individually.

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- Hamiltonian is number preserving for each type of fermion individually.
- Can encode each fermion “separately”, and “stack” copies of encodings together.

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Using Hamiltonian Structure for Better Trotter Error

- Childs *et al.* (2019)¹: improve error bounds to account for commutators: $\|e^{-iHt} - \mathcal{P}(t)\| \leq O(\alpha t^2 \epsilon^{-1})$

$$H = \sum_{\gamma} H_{\gamma} \quad \alpha = \sum_{\gamma_2, \gamma_1}^{\Gamma} \| [H_{\gamma_2}, H_{\gamma_1}] \| \quad (\text{we use similar bounds for } p=2)$$

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- Take advantage of the pionless EFT's number preserving properties

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- Combine this with physical constraints on the systems (e.g. preserved particle number as per Su, Huang & Campbell (2020)²):

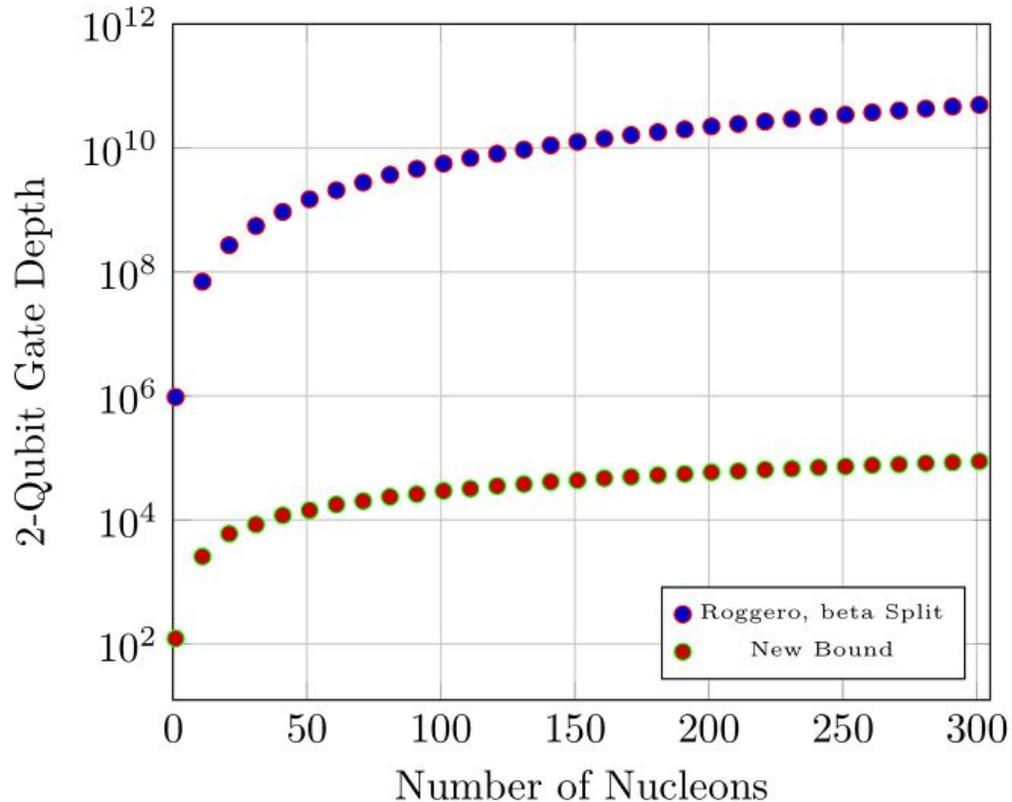
$$\alpha = O(\# \text{ of particles})$$

Comparisons

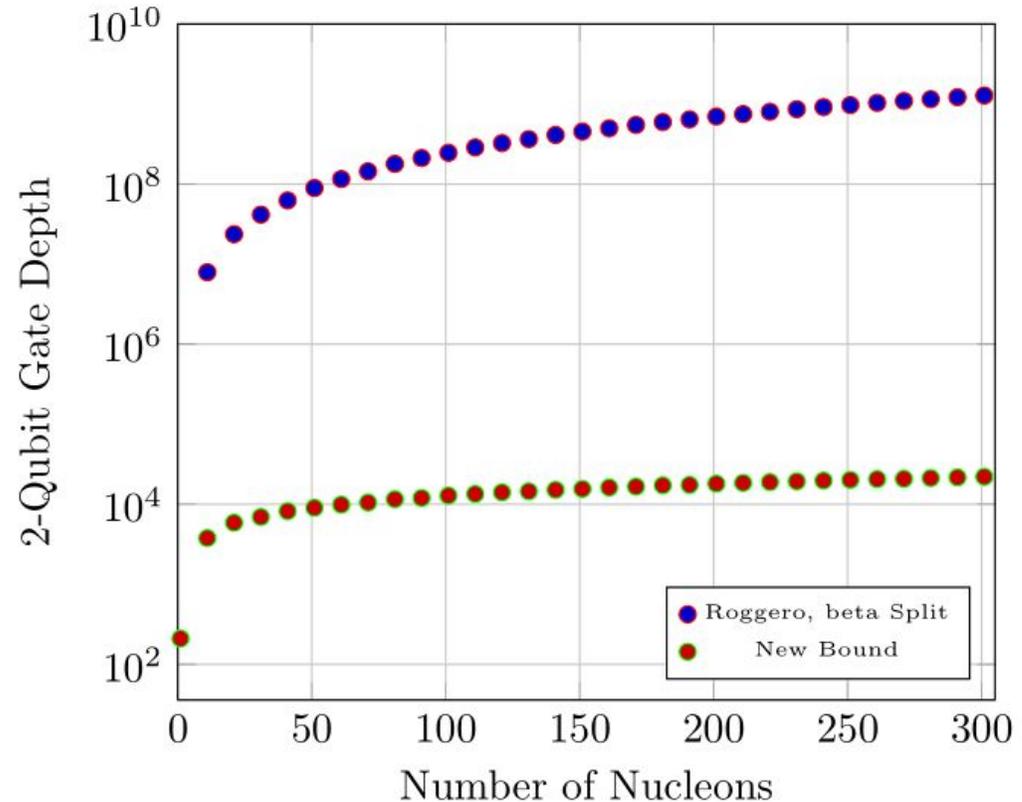


- Comparison for $p=1,2$ Trotter formula having applied these VC encoding + error bounds vs. Roggero *et al.* (2019)¹:

2-Qubit Gate Depth for Time Simulation
for $p = 1$ Product Formula



2-Qubit Gate Depth for Time Simulation
for $p = 2$ Product Formula

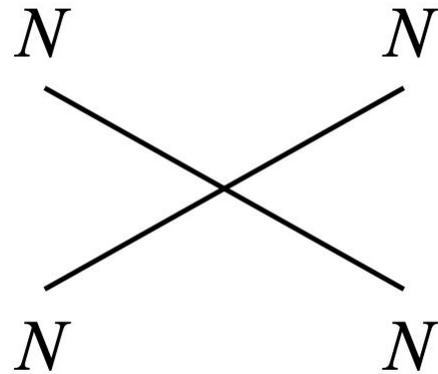




Beyond Pionless EFT

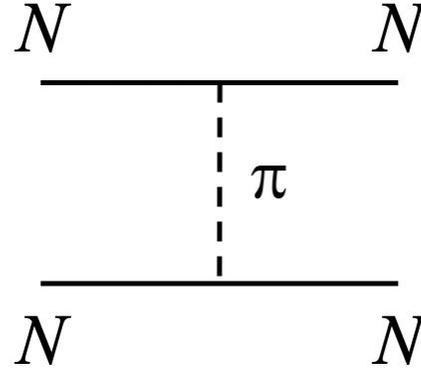
Beyond Pionless EFT

- We now include the first order term



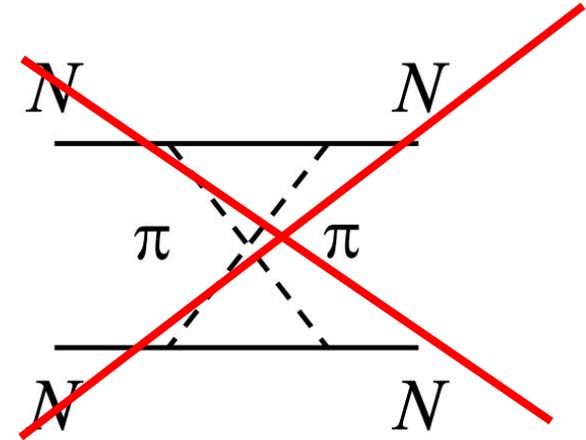
Contact Interactions

+



Single Pion Exchange

+



Two Pion Exchange

Beyond Pionless EFT



- Pionless EFT approximates low-energy Hamiltonian.
- We can include higher order interactions:

$$\mathcal{L}_0 = \frac{1}{2} \partial_\mu \pi_i \partial^\mu \pi_i - \frac{1}{2} m_\pi^2 \pi_i^2$$

Pion Only Terms

$$+ N^\dagger \left[\frac{\nabla^2}{2M} - M \right] N$$

$$- \frac{1}{2} C_S (N^\dagger N) (N^\dagger N) - \frac{1}{2} C_T (N^\dagger \sigma_i N) (N^\dagger \sigma_i N)$$

Nucleon Only Terms

$$+ N^\dagger \left[- \frac{1}{4f_\pi^2} \epsilon_{ijk} \tau_i \pi_j \partial_0 \pi_k - \frac{g_A}{2f_\pi} \tau_i \sigma_j \partial_j \pi_i \right] N$$

Nucleon-Pion Interactions

- But what cost do we pay in simulating this?

Models we investigate:

- **Dynamical pions:** include and explicitly simulate pions.

$$\mathcal{H}_0 = \underbrace{\frac{1}{2} \partial_0 \pi_i \partial^0 \pi_i + \partial_j \pi_i \partial^j \pi_i + \frac{1}{2} m_\pi^2 \pi_i^2}_{\text{Pion Kinetic Term}} + \underbrace{N^\dagger \left[\frac{1}{4f_\pi^2} \epsilon_{ijk} \tau_i \pi_j \partial_0 \pi_k + \frac{g_A}{2f_\pi} \tau_i \sigma^j \partial_j \pi_j \right]}_{\text{Nucleon-Pion Interaction}} N$$

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- **Instantaneous pions:** include pions, but remove their dynamics.

$$\mathcal{H}_0 = \underbrace{\frac{1}{2} \partial_j \pi_i \partial^j \pi_i + \frac{1}{2} m_\pi^2 \pi_i^2}_{\text{Kinetic Term with } \partial_0 \pi_i \text{ removed}} + \underbrace{N^\dagger \left[\frac{g_A}{2f_\pi} \tau_i \sigma^j \partial_j \pi_j \right]}_{\text{Interaction terms with } \partial_0 \pi_i \text{ removed}} N$$

(simulation requires additional Monte Carlo runs)

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(simulation requires additional Monte Carlo runs)

- **One pion exchange:** remove explicit pions and introduce a Yukawa-type potential between fermions.

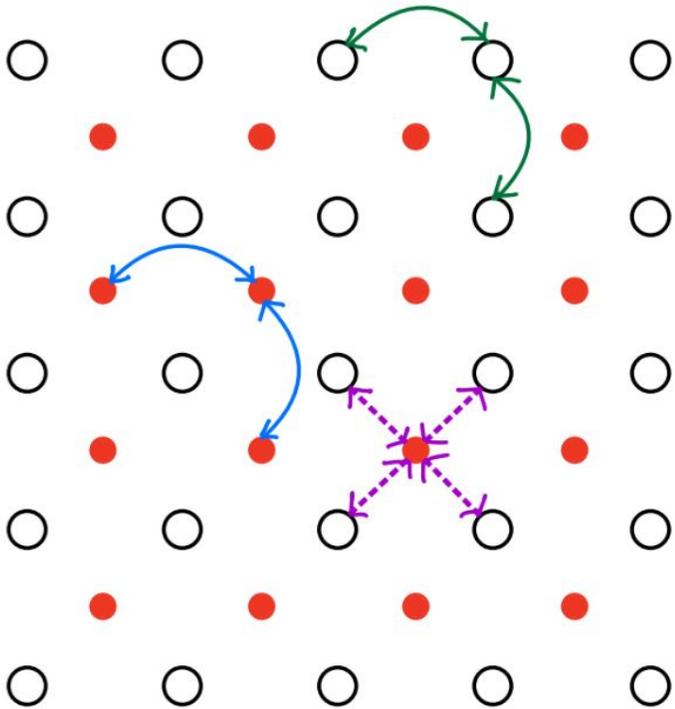
$$V(r) = \frac{1}{4\pi} \left(\frac{g_A}{2f_\pi} \right)^2 \sum_{x,y} [\tau^\mu]_{ik} [\tau^\mu]_{\alpha\gamma} \left[m_\pi^2 \frac{e^{-m_\pi r}}{r} \left\{ S_{12} \left(1 + \frac{3}{m_\pi r} + \frac{3}{m_\pi^2 r^2} \right) + [\sigma^\nu]_{jl} [\sigma^\nu]_{\beta\delta} \right\} - \frac{4\pi}{3} [\sigma^\nu]_{jl} [\sigma^\nu]_{\beta\delta} \delta_{xy} \right] a_{ij}^\dagger(x) a_{\alpha\beta}^\dagger(y) a_{kl}(x) a_{\gamma\beta}(y) \sim \frac{e^{-m_\pi r}}{r}$$

Beyond Pionless EFT



For discretised Hamiltonians, see: Lee (2008)¹ and Madeira *et al.* (2018)²

Dynamical Pions



Hollow circles: fermionic sites.
Red circles: bosonic sites.

Instantaneous Pions

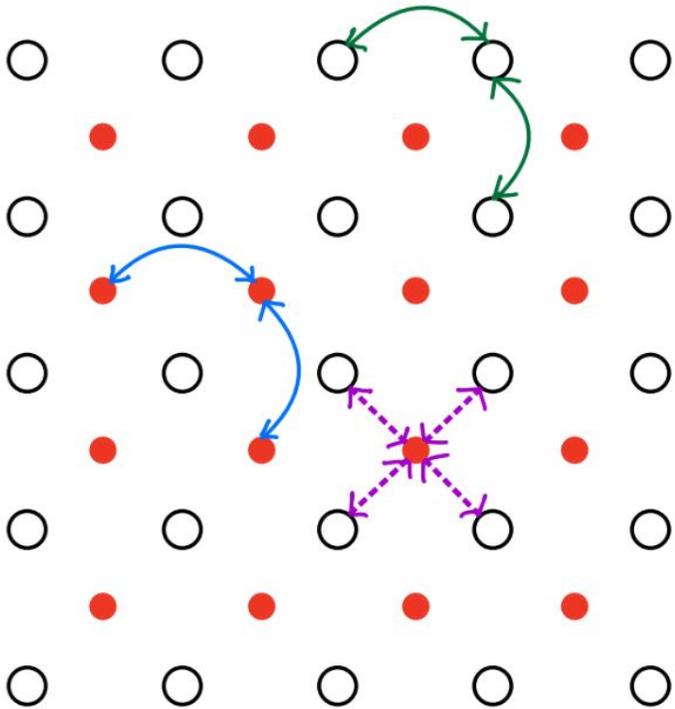
Long-Ranged Interaction

Beyond Pionless EFT



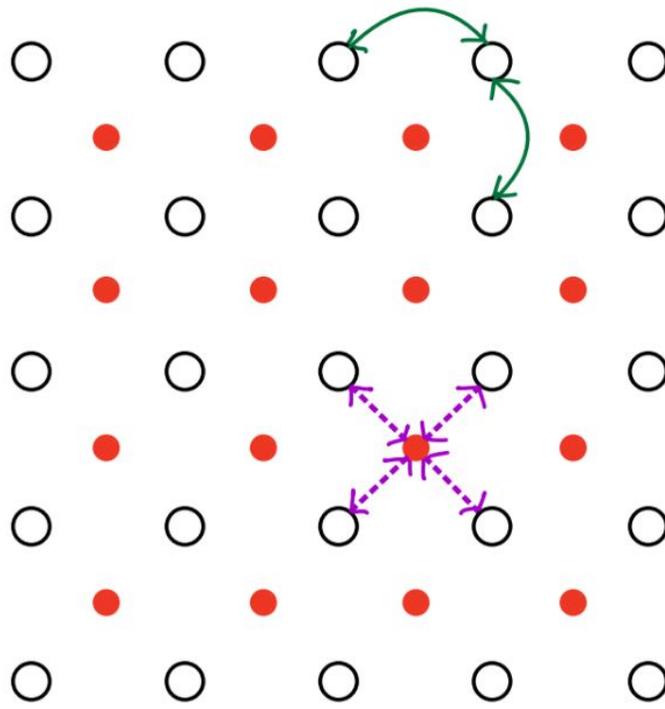
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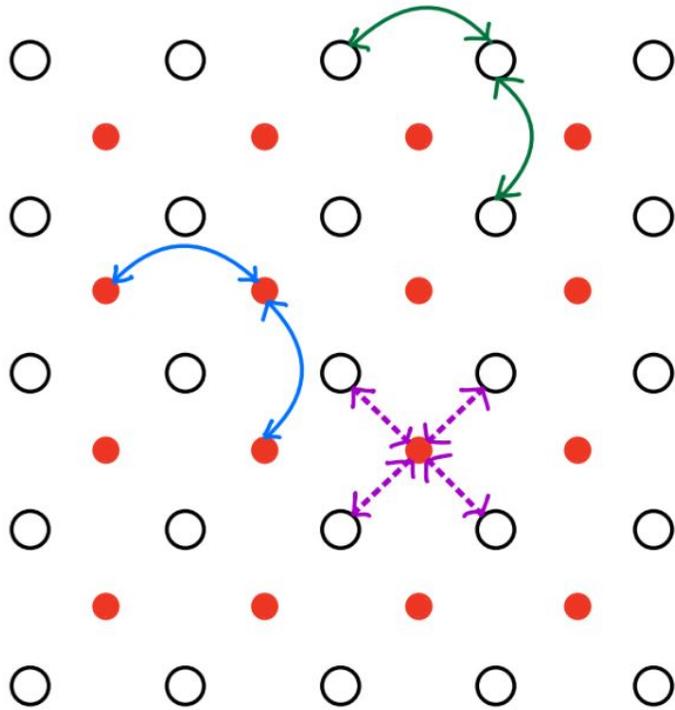
Monte Carlo samples are taken over boson field configurations

Long-Ranged Interaction

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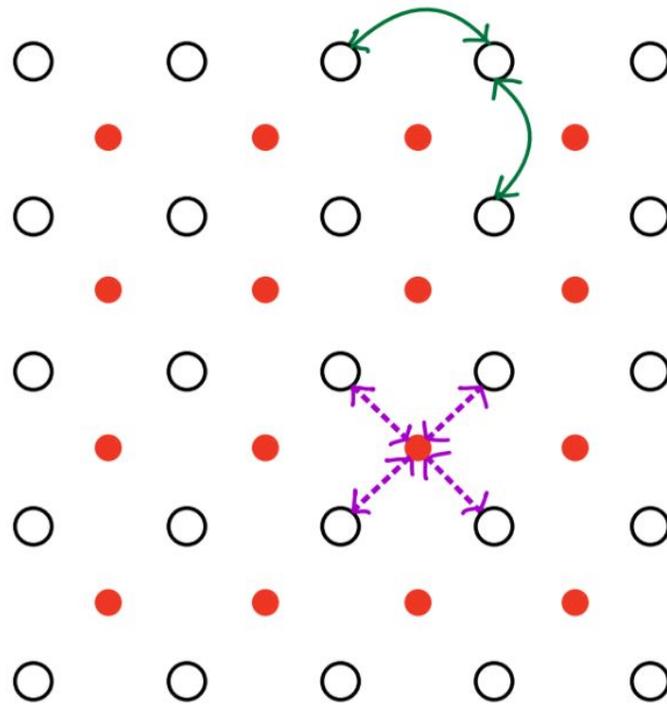
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Dynamical Pions



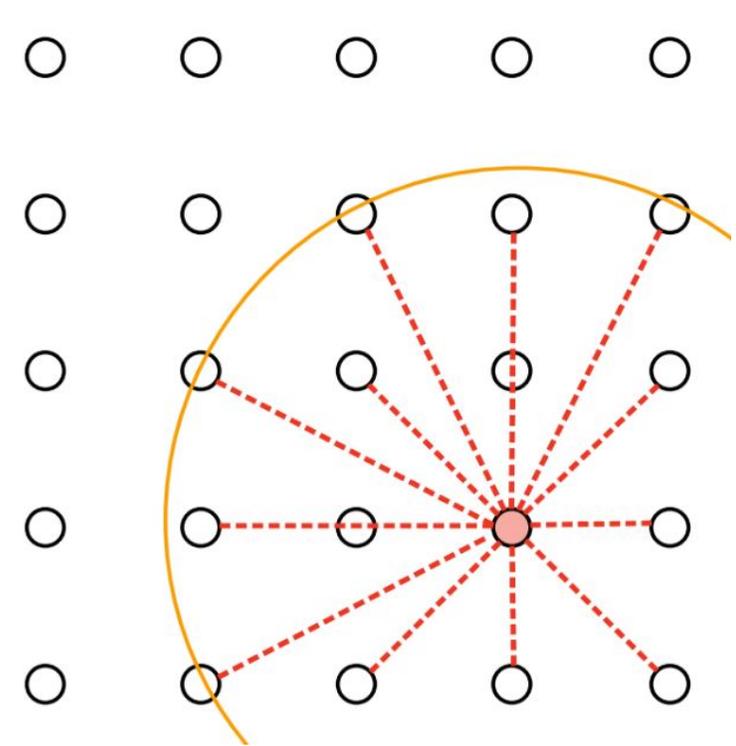
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Instantaneous Pions



Monte Carlo samples are taken over boson field configurations

Long-Ranged Interaction



Models we investigate:

- Dynamical and instantaneous case:
 - Requires explicit encoding of scalar field theory + fermion interactions.
 - See work by Jordan, Lee & Preskill (2012)¹, Klco & Savage (2018)² for scalar fields.
 - Need to:
 - Choose pion basis to minimise circuit depth.
 - Choose pion field representation as spin operators.
 - Choose pion field and conjugate momentum cut-off.
- One Pion Exchange case:
 - Determine best representation for interaction given the fermionic encoding.
 - Determining a cut-off length for the long-ranged interaction.
- Both:
 - Circuit decompositions, Hamiltonian decompositions, etc.



Resource Costs for Spectroscopy

Cost Estimates for Quantum Phase Estimation



- Using the standard quantum phase estimation algorithm and $p=1$ product formulae: 1MeV of energy precision for 6 fermions, on $10 \times 10 \times 10$ lattice, with correctness probability $p > 0.3$.

Model	2-Qubit Gate Depth	T-Gate Cost	T-Gate Time Generation
Pionless			
OPE (Long-Ranged)			
Instantaneous Pions			
Dynamical Pions			

T-gate generation time from "Quantum computation with realistic magic state factories", O'Gorman and Campbell, 2016.

- State preparation step not included!

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Model	2-Qubit Gate Depth	T-Gate Cost	T-Gate Time Generation
Pionless	2×10^7		
OPE (Long-Ranged)	4×10^{17}		
Instantaneous Pions	3×10^{25}		
Dynamical Pions	1×10^{38}		

T-gate generation time from "Quantum computation with realistic magic state factories", O'Gorman and Campbell, 2016.

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Model	2-Qubit Gate Depth	T-Gate Cost	T-Gate Time Generation
Pionless	2×10^7	1×10^{17}	$3 \times 10^3 - 3 \times 10^5$ years
OPE (Long-Ranged)	4×10^{17}	2×10^{28}	$10^{14} - 10^{16}$ years
Instantaneous Pions	3×10^{26}	9×10^{30}	$10^{16} - 10^{18}$ years
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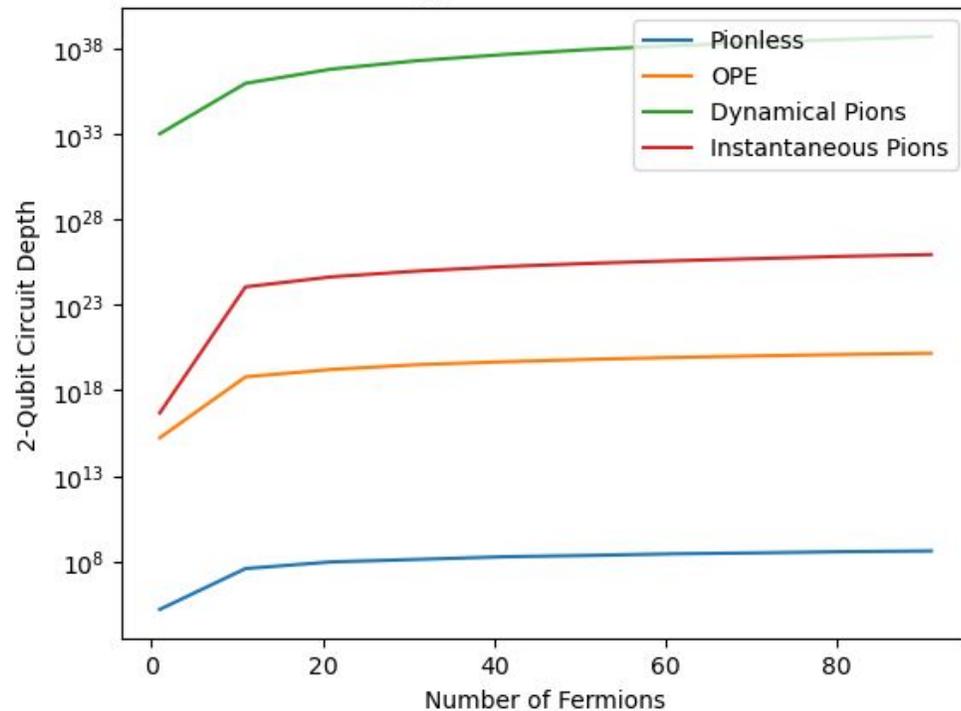
- Current NISQ devices are nowhere near achieving this:
 - Google's Quantum Supremacy Experiment had depth ~ 30 .
 - IBM currently claims depth ~ 100 .

Cost Estimates for Quantum Phase Estimation

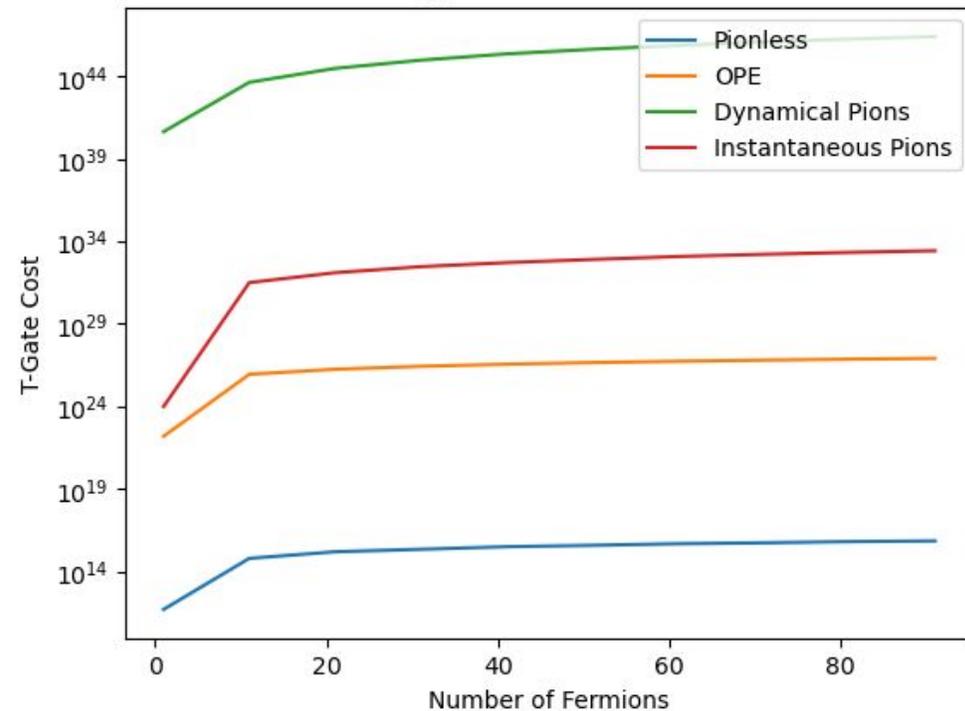


- Using the standard quantum phase estimation algorithm and $p=1$ product formulae: 1MeV of energy precision, on $10 \times 10 \times 10$ lattice, with correctness probability $p > 0.3$.

Phase Estimation Circuit Depths for Different EFTs using $p=1$ Product Formula



Phase Estimation T-Gate Counts for Different EFTs using $p=1$ Product Formula



Asymptotic Scaling



- Scaling of resources for time-simulation with p^{th} order product formula **for fixed time:**

η	Number of fermions	E	Energy Scale
L	Lattice size	ϵ	Precision

Model	2-Qubit Gate Depth	T-Gate Costs	Number of Qubits
Pionless	$O\left(\frac{\eta^{1/p}}{\epsilon^{1/p}}\right)$	$O\left(\frac{\eta^{1/p} L^3}{\epsilon^{1/p}} \log(\eta^{1/p} L^3 / \epsilon^{1/p})\right)$	$O(L^3)$
OPE (Long-Ranged)	$O\left(\frac{\eta^{1/p}}{\epsilon^{1/p}}\right)$	$O\left(\frac{\eta^{1/p} L^3}{\epsilon^{1/p}} \log(\eta^{1/p} L^3 / \epsilon^{1/p})\right)$	$O(L^3)$
Instantaneous Pions	$\tilde{O}\left(\left(\frac{E^2 L^9 \eta^3}{\epsilon^3}\right)^{1/p}\right)$	$\tilde{O}\left(\left(\frac{E^2 L^{12} \eta^3}{\epsilon^3}\right)^{1/p}\right)$	$O(L^3 \log(\eta^2 L^3 E / \epsilon^2))$
Dynamical Pions	$\tilde{O}\left(\left(\frac{E^2 L^9 \eta^4}{\epsilon^3}\right)^{1/p}\right)$	$\tilde{O}\left(\left(\frac{E^2 L^{12} \eta^4}{\epsilon^3}\right)^{1/p}\right)$	$O(L^3 \log(\eta^3 L^3 E / \epsilon^2))$

Cost Estimates for Quantum Phase Estimation



Model	2-Qubit Gate Depth	T-Gate Cost	T-Gate Time Generation
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Conclusions

- Without major improvements to hardware or algorithm, spectroscopy looks unfeasible for NISQ devices.
- OPE and Instantaneous pion models achieve similar efficiencies.
- Dynamical pion models are significantly more expensive than others.

- Examined the task of time evolution and spectroscopy for 4 Chiral Effective Field Theories.
- For Pionless EFT model, utilising Hamiltonian details allows for 10^4 - 10^6 better circuit depths using new techniques.
- Provided the first resource estimates for higher order terms in Effective Field Theory.
- Demonstrated a trade-off between different approximations to the first order terms.
- However, all are infeasible for the near/mid-term.

Maybe there's some hope...



Successive improvements have been found for the Fermi-Hubbard model:

Trotter Bounds	Standard Gate Decompositions	Subcircuit Gate Decompositions
Analytic [Ch+18]	976,710	59,830
Analytic [CBC21]	77,236	1,686
Numerical [CBC21]	3,428	259

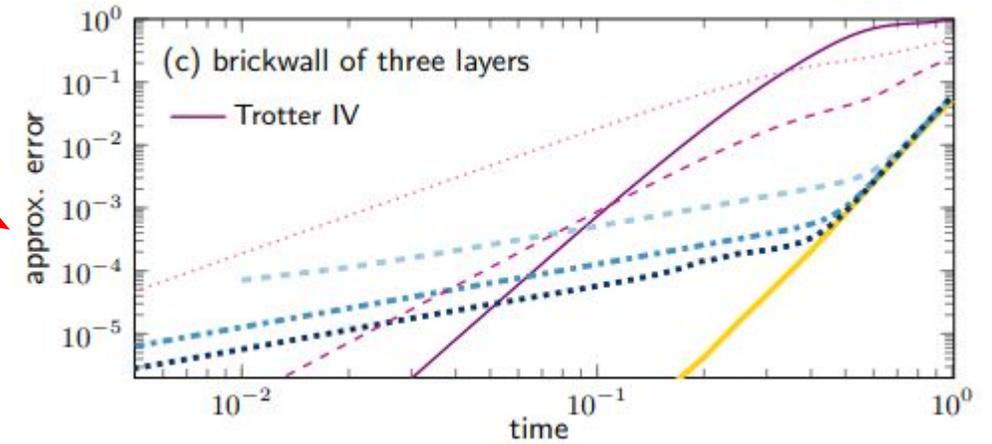
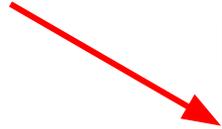
2-qubit gate depth for Fermi-Hubbard model for particular time, error and particle number (Clinton, Bausch, & Cubitt, (2021)¹).

Routes to Improvement



Further improvements we can make:

- Circuit optimisation algorithms.



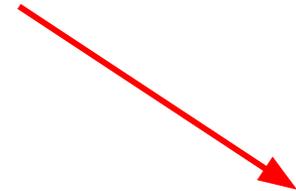
**Error reduction by factor of ~ 100 ,
McKeever & Lubasch, (2022)¹**

Routes to Improvement



Further improvements we can make:

- Circuit optimisation algorithms.
- Non-standard gate decompositions.



Trotter Bounds	Standard	Subcircuit
analytic	77,236	1,686

**Cost reduction by ~10, Clinton,
Bausch & Cubitt, (2020)**

Routes to Improvement



Further improvements we can make:

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- New fermionic encodings?

Fermion encoding	Trotter bounds	Standard decomposition	Subcircuit decomposition
VC	analytic	121,478	95,447
compact	analytic	98,339	72,308

Gate cost reduction from developing new fermionic encoding, Clinton, Bausch, & Cubitt (2020)¹

Routes to Improvement



Further improvements we can make:

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- New fermionic encodings?
- Better phase estimation algorithms.

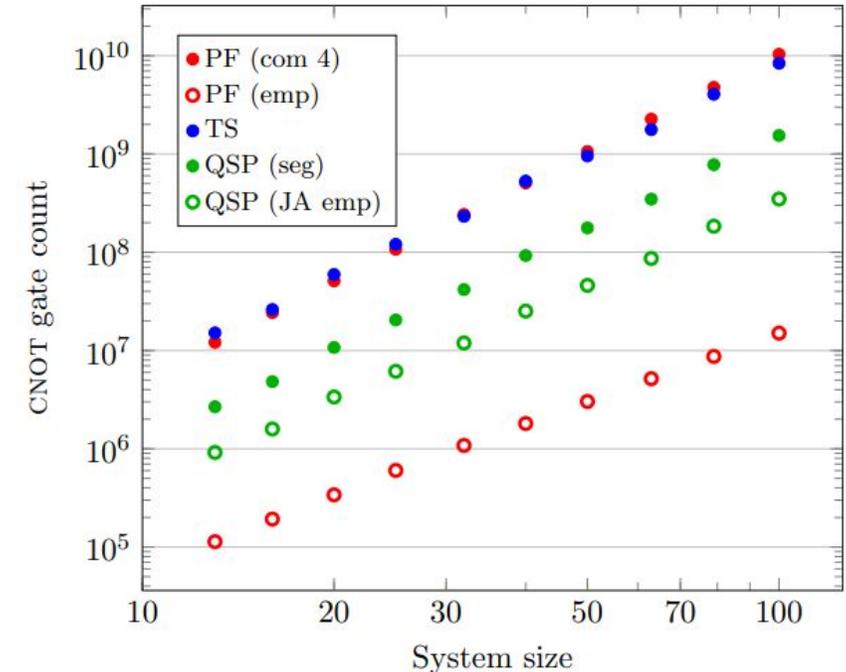
Somma (2020)¹, removes need for controlled unitaries – reduces costs by ~20%.

Routes to Improvement



Further improvements we can make:

- Circuit optimisation algorithms.
- Non-standard gate decompositions.
- New fermionic encodings?
- Better phase estimation algorithms.
- Empirical vs analytical error?



Empirically, the error is often a factor $\sim 10^2$ smaller than the analytical bounds Childs *et al.* (2017)¹.

Routes to Improvement



Further improvements we can make:

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Routes to Improvement



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- Randomised simulation/using Hamiltonian symmetries/etc.

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- T-gate reduction with different hardware models.
- Lower-cost use cases?
- Partial error correcting properties of fermionic encodings?
- Randomised simulation/using Hamiltonian symmetries/etc.
- Other ways of simulating nuclear physics besides lattice EFT formulation?













- Techniques improving quantum algorithms for simulating time evolution of EFTs.
- Beyond pionless EFT & associated costs.

EFTs and Quantum Computing



- First principles nuclear dynamics is difficult – use an effective field theory instead!
- Time evolution is an important primitive, e.g. for quantum phase estimation.

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- Try simulating using product formulae. For Hamiltonian: $H = \sum_{\gamma=1}^L H_{\gamma}$

$$e^{-iH\delta t} \approx e^{-iH_1\delta t} e^{-iH_2\delta t} \dots e^{-iH_L\delta t} =: \mathcal{P}(\delta t)$$

$$\left\| e^{-iH\delta t} - \mathcal{P}(\delta t) \right\| \leq \epsilon$$

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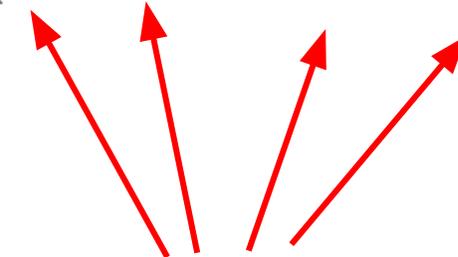
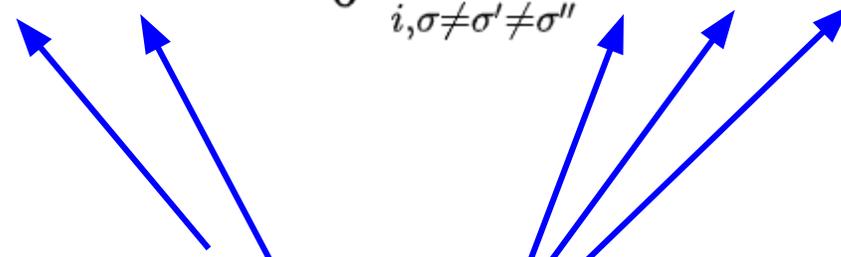
$$\left\| e^{-iH\delta t} - \mathcal{P}(\delta t) \right\| \leq \epsilon$$

- Product formulae have low overhead and generally perform well!
- How well can we improve our error bounds and optimise computational resources?

Previous Work in EFTs and Quantum Computing

Roggero *et al.* (2019)¹ on simulating time evolution and linear response function using pionless effective field theory model.

$$H_{EFT} = \overbrace{\frac{1}{2Ma^2} \sum_{\langle i,j \rangle} \left(a_{\sigma}^{\dagger}(i) a_{\sigma}(j) + a_{\sigma}^{\dagger}(j) a_{\sigma}(i) \right)}^{\text{kinetic term}} + \overbrace{\frac{C}{2} \sum_{i, \sigma \neq \sigma'} n_{\sigma}(i) n_{\sigma'}(i)}^{\text{2-body onsite interaction}} + \overbrace{\frac{D}{6} \sum_{i, \sigma \neq \sigma' \neq \sigma''} n_{\sigma}(i) n_{\sigma'}(i) n_{\sigma''}(i)}^{\text{3-body onsite interaction}}$$

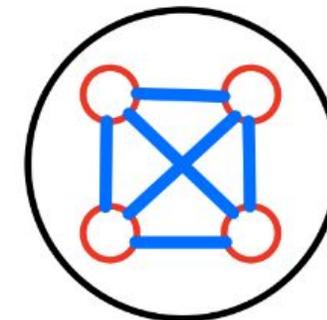
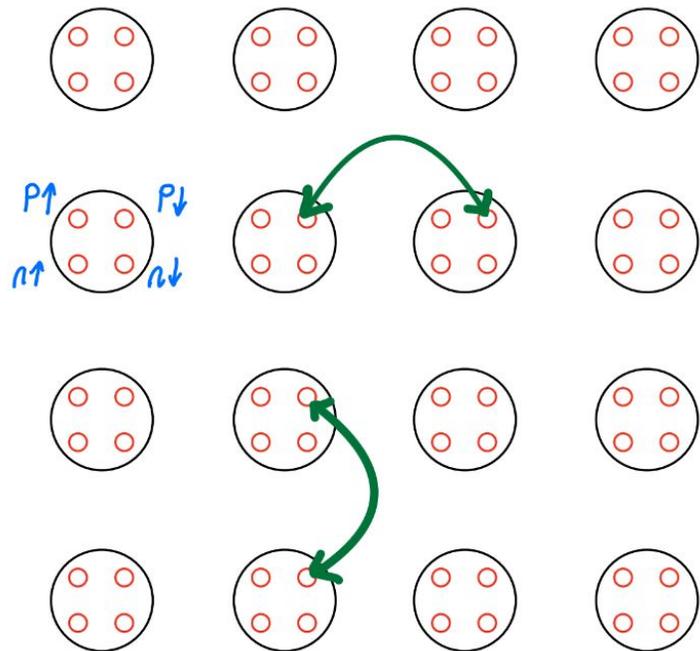



Creation and annihilation operators for nucleons.
 Nucleon number operator at site i .

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$$H_{FH} = \underbrace{J \sum_{\langle i,j \rangle} \left(a_{\sigma}^{\dagger}(i) a_{\sigma}(j) + a_{\sigma}^{\dagger}(j) a_{\sigma}(i) \right)}_{\text{kinetic terms}} + \underbrace{U \sum_{i, \sigma \neq \sigma'} n_{\sigma}(i) n_{\sigma'}(i)}_{\text{2-body onsite interaction}}$$

The Fermi-Hubbard model is similar and well studied – can we apply techniques from its analysis + improved Trotter analysis to get bounds?

Better Trotter Bounds



- Childs *et al.* (2019)¹: improve error bounds to account for commutators: $\|e^{-iHt} - \mathcal{P}(t)\| \leq O(\alpha t^2 \epsilon^{-1})$

$$H = \sum_{\gamma} H_{\gamma} \quad \alpha = \sum_{\gamma_2, \gamma_1}^L \| [H_{\gamma_2}, H_{\gamma_1}] \| \quad (\text{we use similar bounds for } p=2)$$

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- Combine this with physical constraints on the systems (e.g. preserved particle number as per Su, Huang & Campbell (2020)²):

$$\alpha = O(\# \text{ of particles})$$

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- Yi & Crosson(2021)³: improve error for quantum phase estimation by considering the effective Trotterised Hamiltonian.

Better Circuit Depths



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- Due to non-locality of fermions:
 - If fermions are encoded via Jordan-Wigner mapping, this term takes $O(L^{D-1})$ gates to implement.
 - Alternatives: Fast Fermionic Fourier Transform/SWAP Network/Givens Rotation, need gate depth proportional to number of fermionic modes.

Better Circuit Depths



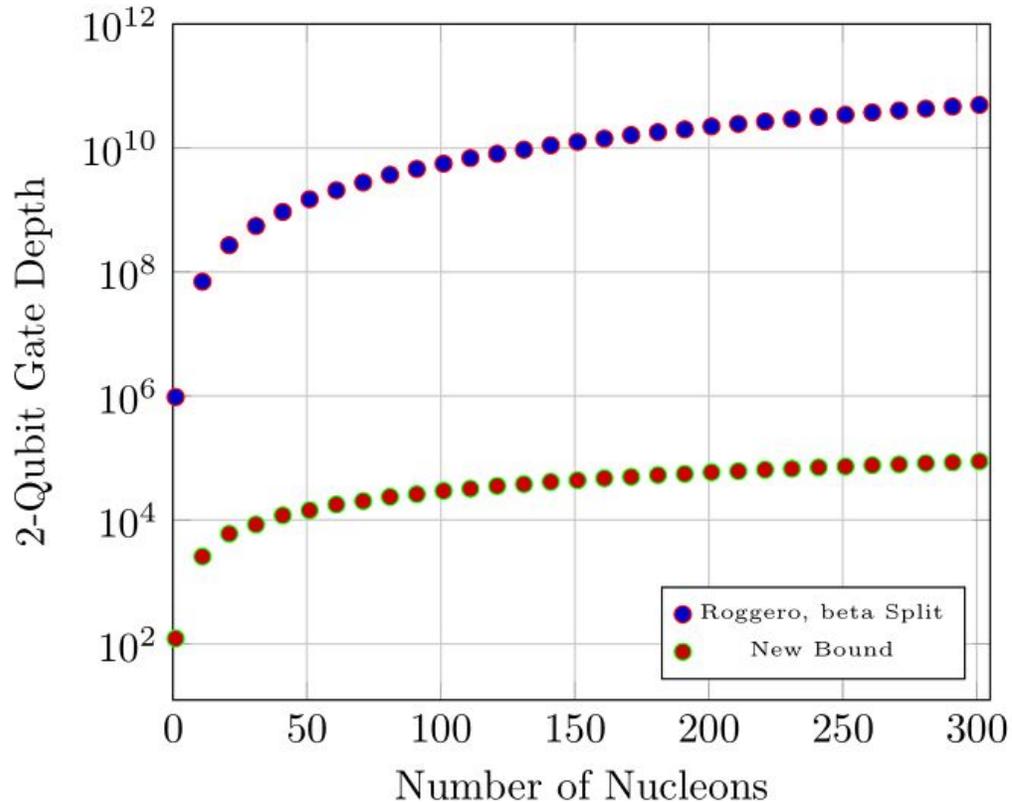
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 - Alternatives: Fast Fermionic Fourier Transform/SWAP Network/Givens Rotation, need gate depth proportional to number of fermionic modes.
- Leverage interaction locality: encode fermions using Verstraete-Cirac encoding.
 - Implement in circuit of depth ~ 100 , regardless of number of fermions or lattice size.

Comparisons

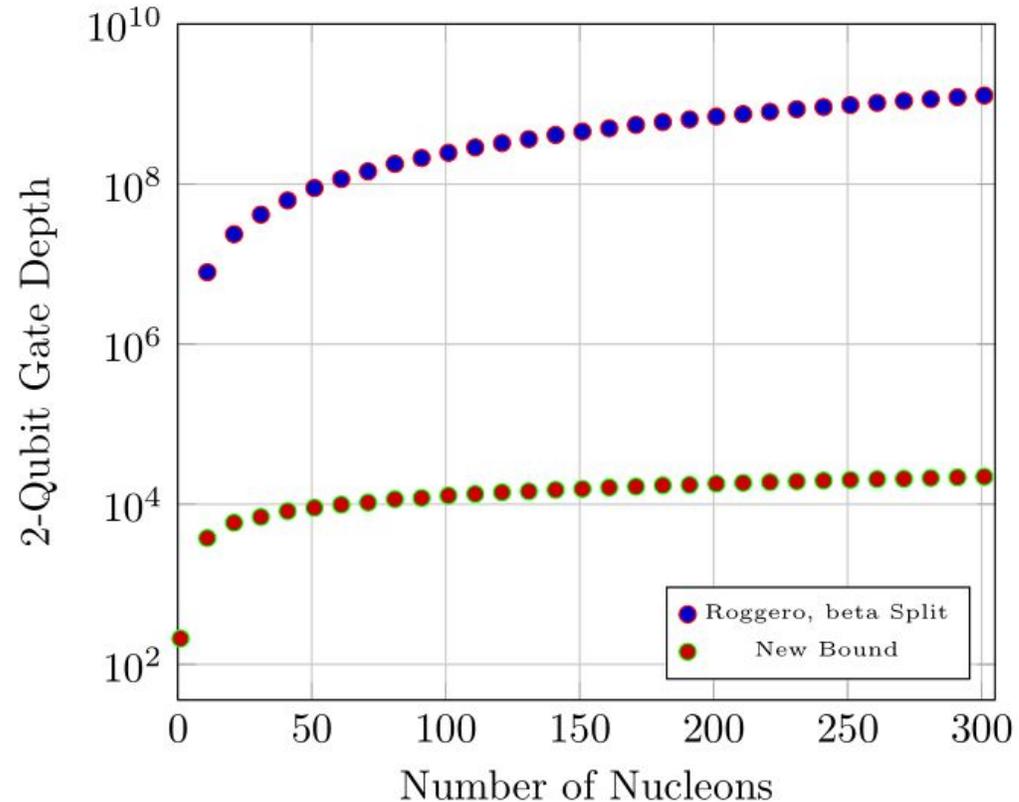


- Comparison for $p=1,2$ Trotter formula having applied these methods vs. bounds from Roggero *et al.* (2019)¹:

2-Qubit Gate Depth for Time Simulation
for $p = 1$ Product Formula



2-Qubit Gate Depth for Time Simulation
for $p = 2$ Product Formula





Beyond Pionless EFT

Beyond Pionless EFT



- Pionless EFT approximates low-energy Hamiltonian.
- We can include higher order interactions:

$$\mathcal{L}_0 = \frac{1}{2} \partial_\mu \pi_i \partial^\mu \pi_i - \frac{1}{2} m_\pi^2 \pi_i^2$$

Pion Only Terms

$$+ N^\dagger \left[\frac{\nabla^2}{2M} - M \right] N$$

$$- \frac{1}{2} C_S (N^\dagger N) (N^\dagger N) - \frac{1}{2} C_T (N^\dagger \sigma_i N) (N^\dagger \sigma_i N)$$

Nucleon Only Terms

$$+ N^\dagger \left[- \frac{1}{4f_\pi^2} \epsilon_{ijk} \tau_i \pi_j \partial_0 \pi_k - \frac{g_A}{2f_\pi} \tau_i \sigma_j \partial_j \pi_i \right] N$$

Nucleon-Pion Interactions

- But what cost do we pay in simulating this?

Models we investigate:

- **Dynamical pions:** include and explicitly simulate pions.

$$\mathcal{H}_0 = \underbrace{\frac{1}{2} \partial_0 \pi_i \partial^0 \pi_i + \partial_j \pi_i \partial^j \pi_i + \frac{1}{2} m_\pi^2 \pi_i^2}_{\text{Pion Kinetic Term}} + \underbrace{N^\dagger \left[\frac{1}{4f_\pi^2} \epsilon_{ijk} \tau_i \pi_j \partial_0 \pi_k + \frac{g_A}{2f_\pi} \tau_i \sigma^j \partial_j \pi_j \right]}_{\text{Nucleon-Pion Interaction}} N$$

Models we investigate:

- **Dynamical pions:** include and explicitly simulate pions.

$$\mathcal{H}_0 = \underbrace{\frac{1}{2} \partial_0 \pi_i \partial^0 \pi_i + \partial_j \pi_i \partial^j \pi_i + \frac{1}{2} m_\pi^2 \pi_i^2}_{\text{Pion Kinetic Term}} + \underbrace{N^\dagger \left[\frac{1}{4f_\pi^2} \epsilon_{ijk} \tau_i \pi_j \partial_0 \pi_k + \frac{g_A}{2f_\pi} \tau_i \sigma^j \partial_j \pi_j \right]}_{\text{Nucleon-Pion Interaction}} N$$

- **Instantaneous pions:** include pions, but remove their dynamics.

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- **One pion exchange:** remove explicit pions and introduce an effective Yukawa-type potential between fermions.

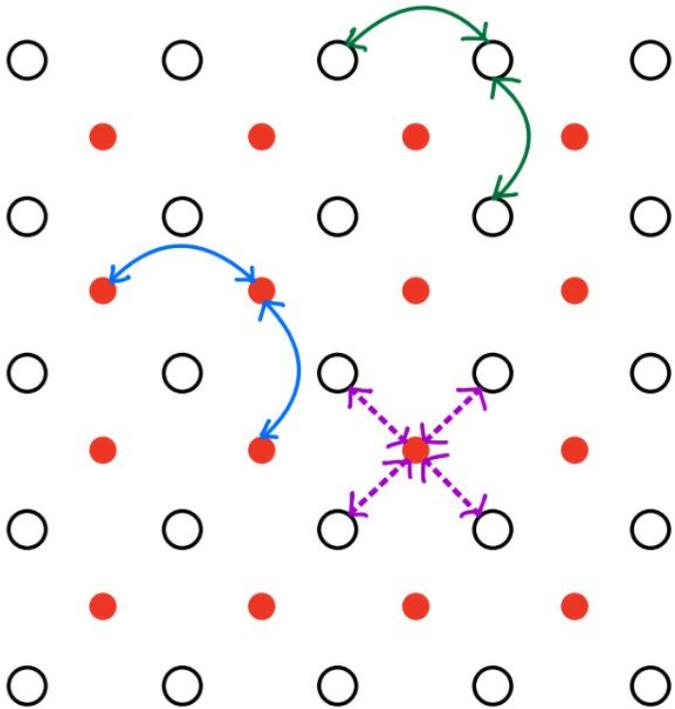
$$V(r) = \frac{1}{4\pi} \left(\frac{g_A}{2f_\pi} \right)^2 \sum_{x,y} [\tau^\mu]_{ik} [\tau^\mu]_{\alpha\gamma} \left[m_\pi^2 \frac{e^{-m_\pi r}}{r} \left\{ S_{12} \left(1 + \frac{3}{m_\pi r} + \frac{3}{m_\pi^2 r^2} \right) + [\sigma^\nu]_{jl} [\sigma^\nu]_{\beta\delta} \right\} - \frac{4\pi}{3} [\sigma^\nu]_{jl} [\sigma^\nu]_{\beta\delta} \delta_{xy} \right] a_{ij}^\dagger(x) a_{\alpha\beta}^\dagger(y) a_{kl}(x) a_{\gamma\beta}(y) \sim \frac{e^{-m_\pi r}}{r}$$

Beyond Pionless EFT



For discretised Hamiltonians, see: Lee (2008)¹ and Madeira *et al.* (2018)²

Dynamical Pions



Hollow circles: fermionic sites.
Red circles: bosonic sites.

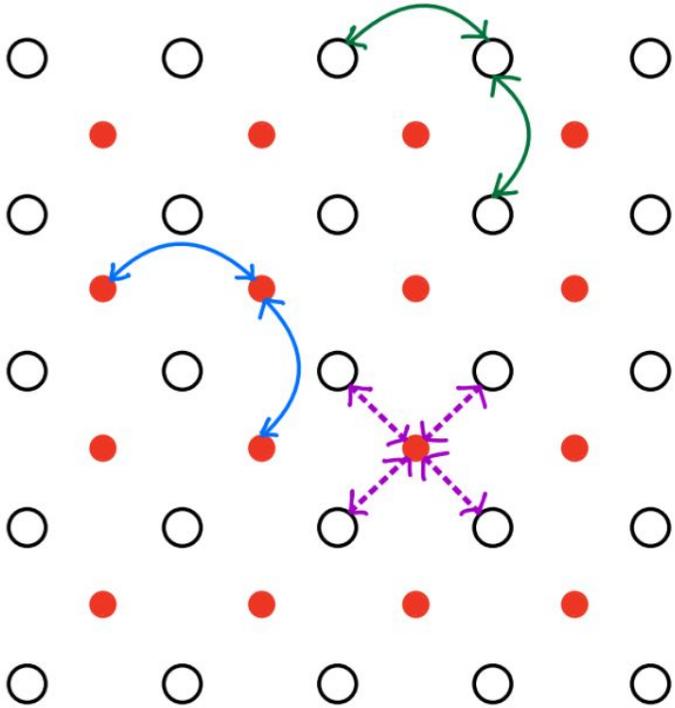
Instantaneous Pions

Long-Ranged Interaction

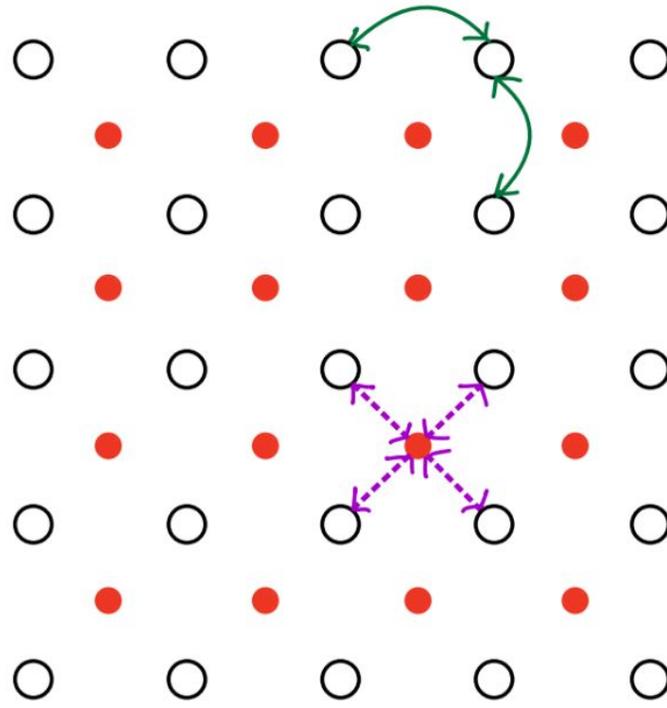
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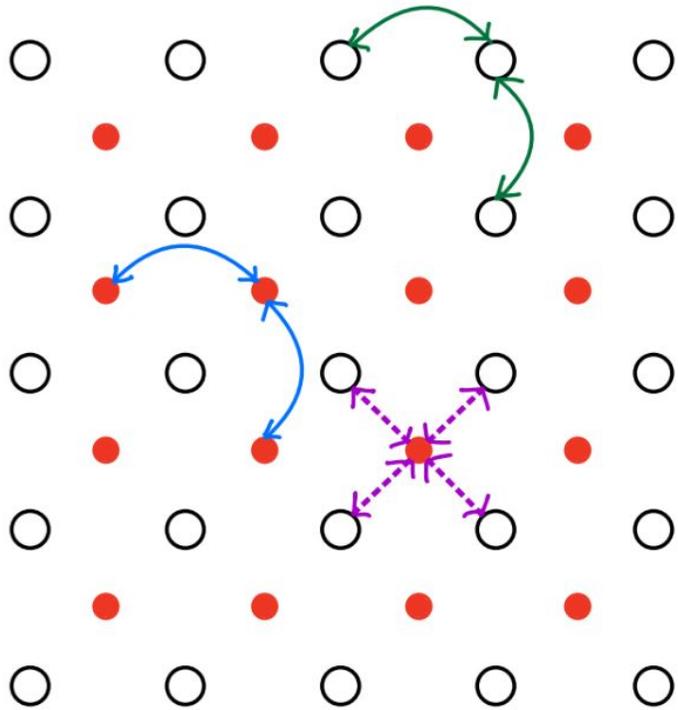
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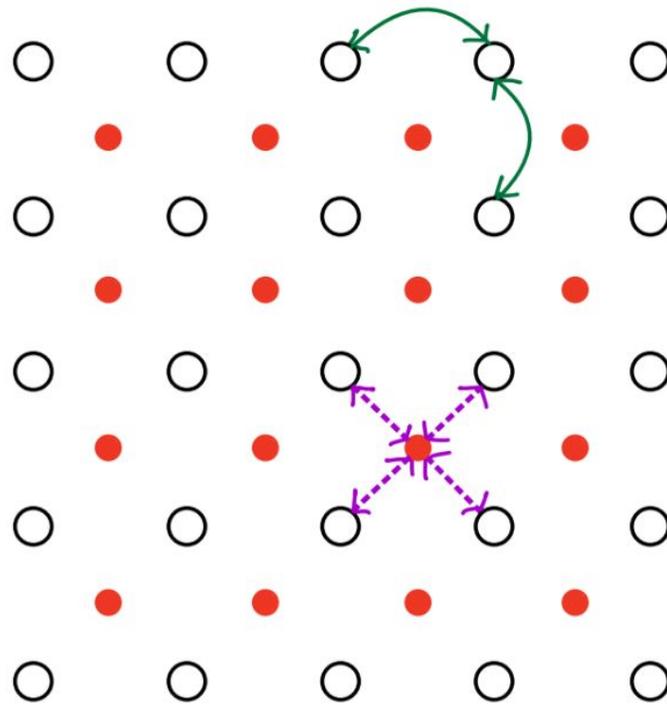
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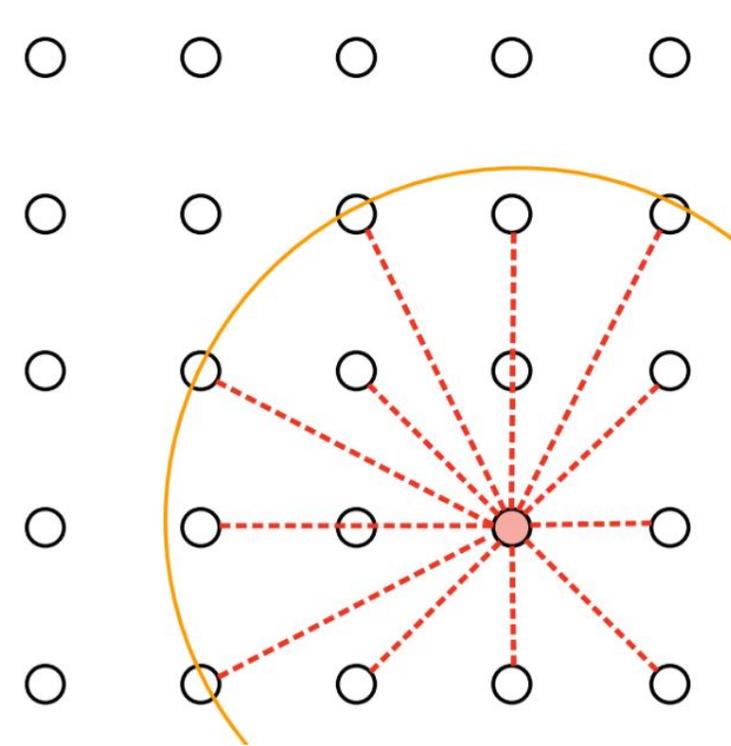
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Models we investigate:

- Dynamical and instantaneous case:
 - Requires explicit encoding of scalar field theory + fermion interactions.
 - See work by Jordan, Lee & Preskill (2012)¹, Klco & Savage (2018)² for scalar fields.
 - Need to:
 - Choose pion basis to minimise circuit depth.
 - Choose pion field representation as spin operators.
 - Choose pion field and conjugate momentum cut-off.

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 - Choose pion field representation as spin operators.
 - Choose pion field and conjugate momentum cut-off.
- One Pion Exchange case:
 - Determine best representation for interaction given the fermionic encoding.
 - Determining a cut-off length for the long-ranged interaction.

Cost Estimates for Quantum Phase Estimation



- Using the standard quantum phase estimation algorithm and $p=1$ product formulae: 1MeV of energy precision for 6 fermions, on $10 \times 10 \times 10$ lattice, with correctness probability $p > 0.9$.

Model	2-Qubit Gate Depth	T-Gate Cost	T-Gate Time Generation
Pionless			
OPE			
Instantaneous Pions			
Dynamical Pions			

T-gate generation time from "Quantum computation with realistic magic state factories", O'Gorman and Campbell, 2016.

- State preparation step not included!

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- Current NISQ devices are nowhere near achieving this:
 - Google's Quantum Supremacy Experiment had depth ~ 30 .
 - IBM currently claims depth ~ 100 .

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- Additional question: what is the "correct" precision to work to for each model? High precision pointless if the effective Hamiltonian has larger systematic error.

Maybe there's some hope...



Successive improvements have been found for the Fermi-Hubbard model:

Trotter Bounds	Standard Gate Decompositions	Subcircuit Gate Decompositions
Analytic [Ch+18]	976,710	59,830
Analytic [CBC21]	77,236	1,686
Numerical [CBC21]	3,428	259

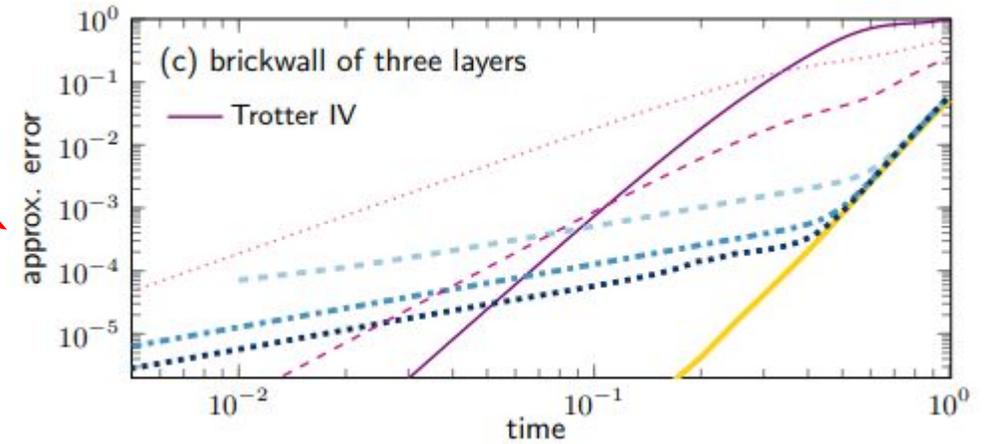
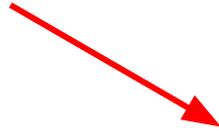
2-qubit gate depth for Fermi-Hubbard model for particular time, error and particle number (Clinton, Bausch, & Cubitt, (2021)¹).

Routes to Improvement



Further improvements we can make:

- Circuit optimisation algorithms.



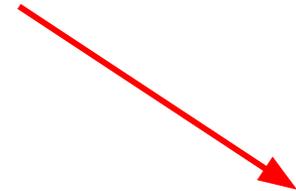
**Error reduction by factor of ~ 100 ,
McKeever & Lubasch, (2022)¹**

Routes to Improvement



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Trotter Bounds	Standard	Subcircuit
analytic	77,236	1,686

**Cost reduction by ~10, Clinton,
Bausch & Cubitt, (2020)**

Routes to Improvement



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- New fermionic encodings?

Fermion encoding	Trotter bounds	Standard decomposition	Subcircuit decomposition
VC	analytic	121,478	95,447
compact	analytic	98,339	72,308

Gate cost reduction from developing new fermionic encoding, Clinton, Bausch, & Cubitt (2020)¹

Routes to Improvement



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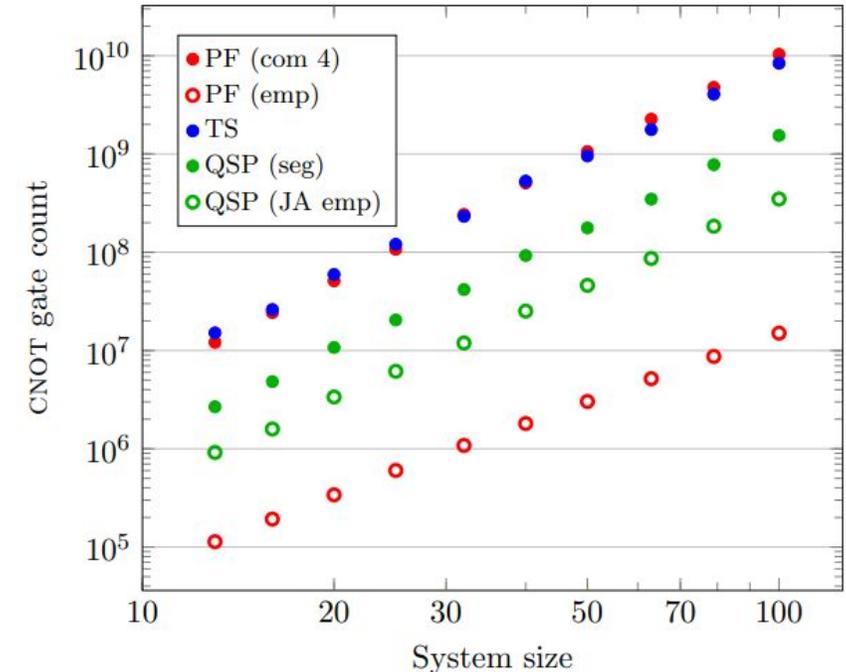
Somma (2020)¹, removes need for controlled unitaries – reduces costs by ~20%.

Routes to Improvement



Further improvements we can make:

- Circuit optimisation algorithms.
- Non-standard gate decompositions.
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- Better phase estimation algorithms.
- Empirical vs analytical error?



Empirically, the error is often a factor $\sim 10^2$ smaller than the analytical bounds Childs *et al.* (2017)¹.

Routes to Improvement



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- Partial error correcting properties of fermionic encodings?
- Randomised simulation/using Hamiltonian symmetries/etc.
- Other ways of simulating nuclear physics besides lattice EFT formulation?







Limitations of New Techniques



- Childs et al error improve bounds to account for commutators:

$$\|e^{-iHt} - \mathcal{P}_p(t)\| \leq O(\alpha t^{1+p} \epsilon^{-p})$$

$$\alpha = \sum_{\gamma_{p+1}, \gamma_p \dots \gamma_1} \| [H_{\gamma_{p+1}}, \dots [H_{\gamma_2}, H_{\gamma_1}]] \|$$

- Calculating nested commutator is difficult for $p > 2$.
- Verstraete-Cirac encoding comes with more difficult state preparation.

Future Work



- Different spectroscopy/QPE algorithms.
- Optimising circuit depths and T-gate counts.
- Non-standard gate decompositions.
- Inherent error correction in fermionic encodings
- Lower-cost use cases generally?



Beyond Pionless EFT



- Pionless EFT approximates low-energy Hamiltonian.
- We can include higher order interactions:

$$\begin{aligned}\mathcal{L}_0 = & \frac{1}{2}\partial_\mu\pi_i\partial^\mu\pi_i - \frac{1}{2}m_\pi^2\pi_i\pi_i + N^\dagger\left[i\partial_0 + \frac{\nabla^2}{2M_0}\right. \\ & \left. - \frac{1}{4f_\pi^2}\epsilon_{ijk}\tau_i\pi_j\partial_0\pi_k - \frac{g_A}{2f_\pi}\tau_i\sigma^j\partial_j\pi_i - M_0\right]N \\ & - \frac{1}{2}C_S(N^\dagger N)(N^\dagger N) - \frac{1}{2}C_T(N^\dagger\sigma_i N)(N^\dagger\sigma_i N)\end{aligned}$$

- But what cost do we pay in simulating this?

- Childs *et al.* (2019)¹: improve error bounds to account for commutators: $\|e^{-iHt} - \mathcal{P}(t)\| \leq O(\alpha t^2 \epsilon^{-1})$

$$H = \sum_{\gamma} H_{\gamma} \quad \alpha = \sum_{\gamma_2, \gamma_1}^L \| [H_{\gamma_2}, H_{\gamma_1}] \| \quad (\text{we use similar bounds for } p=2)$$

- Combine this with physical constraints on the systems (e.g. preserved particle number as per Su, Huang & Campbell (2020)²):

$$\alpha = O(\# \text{ of particles})$$

- Yi & Crosson(2021)³: improve error for quantum phase estimation by considering the effective Trotterised Hamiltonian.

- Pionless EFT is the simplest Hamiltonian that recreates basic properties of the nucleus.

$$H_{EFT} = \overbrace{\frac{1}{2Ma^2} \sum_{\langle i,j \rangle} \left(a_{\sigma}^{\dagger}(i) a_{\sigma}(j) + a_{\sigma}^{\dagger}(j) a_{\sigma}(i) \right)}^{\text{kinetic term}} + \overbrace{\frac{C}{2} \sum_{i, \sigma \neq \sigma'} n_{\sigma}(i) n_{\sigma'}(i)}^{\text{2-body onsite interaction}} + \overbrace{\frac{D}{6} \sum_{i, \sigma \neq \sigma' \neq \sigma''} n_{\sigma}(i) n_{\sigma'}(i) n_{\sigma''}(i)}^{\text{3-body onsite interaction}}$$

$$H_{FH} = \underbrace{J \sum_{\langle i,j \rangle} \left(a_{\sigma}^{\dagger}(i) a_{\sigma}(j) + a_{\sigma}^{\dagger}(j) a_{\sigma}(i) \right)}_{\text{kinetic terms}} + \underbrace{U \sum_{i, \sigma \neq \sigma'} n_{\sigma}(i) n_{\sigma'}(i)}_{\text{2-body onsite interaction}}$$

The Fermi-Hubbard model is similar and well studied – can we apply techniques from its analysis + improved Trotter analysis to get bounds?