Quantum Simulation of Scattering via Hamiltonian Truncation

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Outline

Based on 2505.03878 with M. Spannowsky, T. Sypchenko, S. Williams and M. Wingate

Hamiltonian Truncation Overview

Hamiltonian Setup

$$H = H_0 + V \tag{1}$$

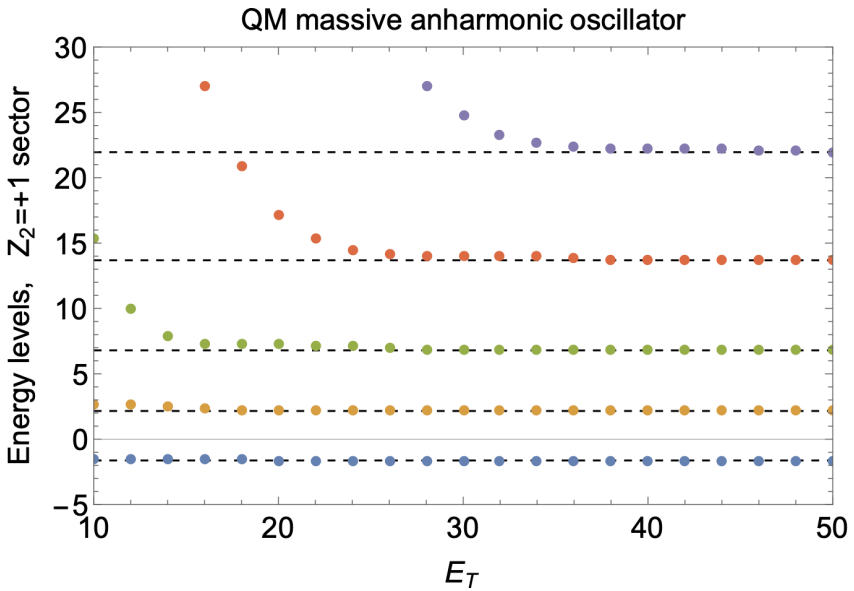
- H_0 is an exactly solvable Hamiltonian
- V represents a new interaction, which may be strong.
- Work in the eigenbasis of H_0. Truncate so that only a finite number of states with $E_0 \leq E_T$ are included in the basis.
- Diagonalize numerically to calculate spectrum and wavefunctions.

A Simple Example: The Anharmonic Oscillator

Take the quantum mechanical model

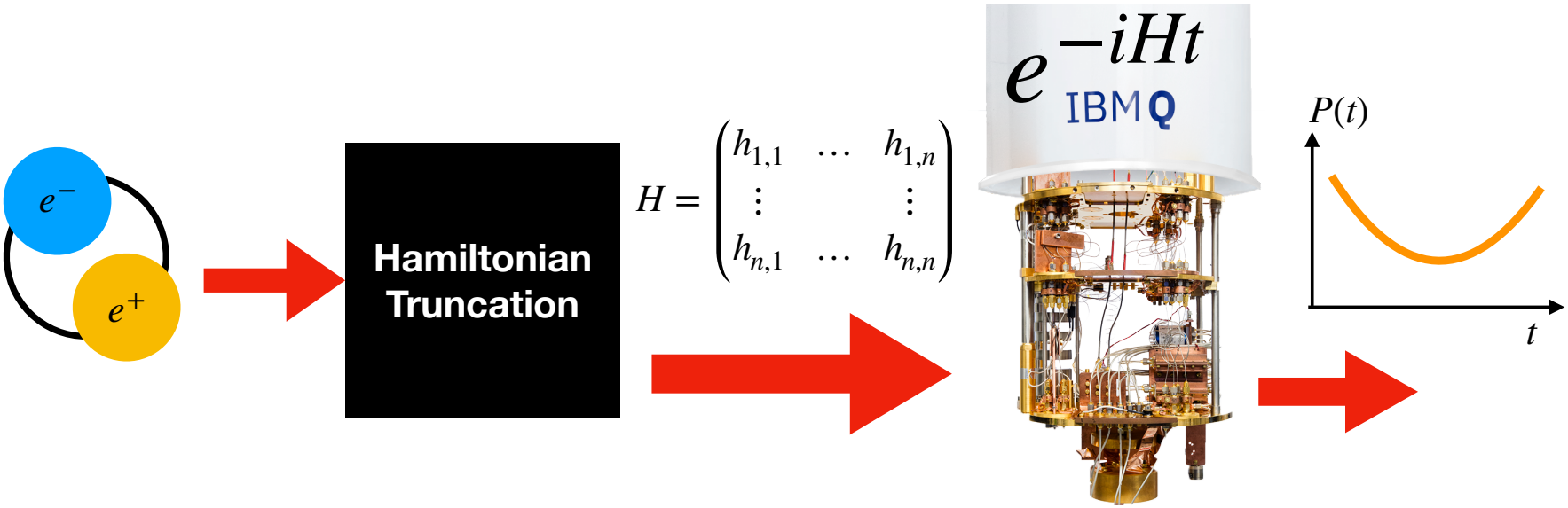
$$H = \frac{p^2 + x^2}{2} + \lambda x^4 \,. \tag{2}$$

Decompose the Hamiltonian so that H_0 is the SHO and $V = \lambda x^4$. Work in the SHO eigenbasis: $H_0 \left|n\right\rangle = (n + 1/2) \left|n\right\rangle$



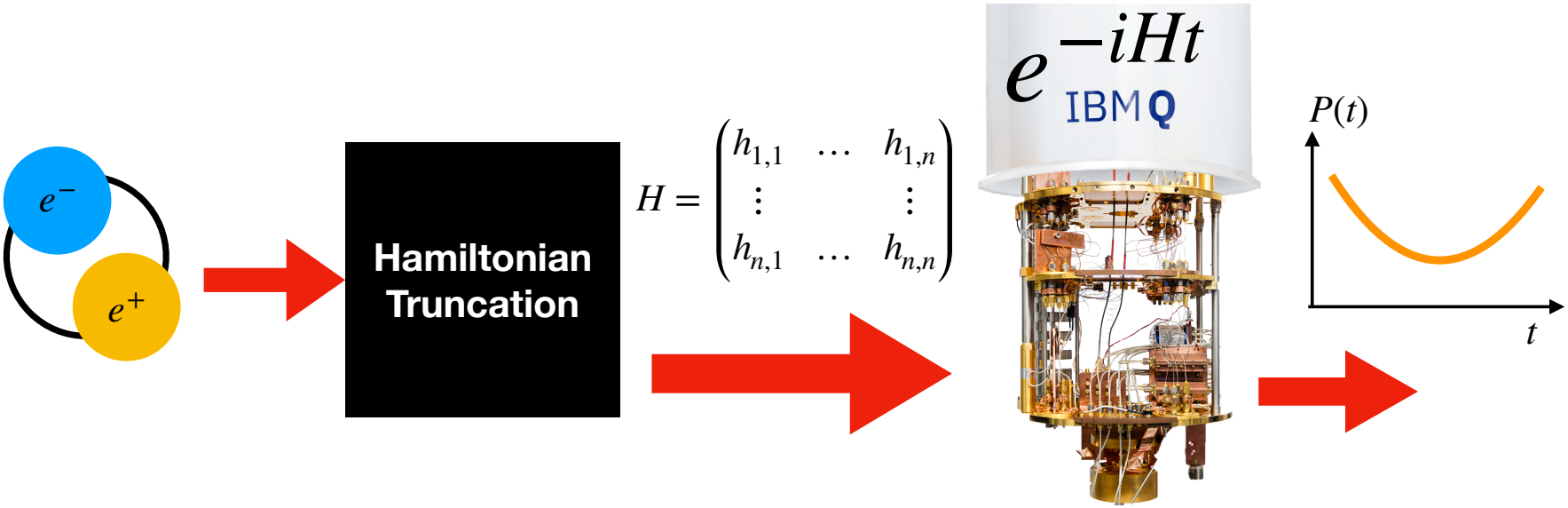
- Truncate basis to include states $\left|n\right\rangle$ for $n + 1/2 \leq E_T$.
- All energy eigenvalues are upper bounds for the true energies due to min-max theorem.
- Method generalises to QFTs.

General Idea



1. We use Hamiltonian Truncation to generate an approximate Hamiltonian for our system of low dimensionality.

General Idea



1. We use Hamiltonian Truncation to generate an approximate Hamiltonian for our system of low dimensionality.
2. We use a qubit based, gate based, quantum device to determine how this probability evolves with time.

ϕ^4 Theory in Hamiltonian Truncation

The HT formulation of ϕ^4 theory in $1+1d$ was developed in [S. Rychkov, L. Vitale '14]

$$H_0 = \frac{1}{2}\int_0^L dx \ :\Pi^2 + (\partial_x \phi)^2 + m^2\phi^2: \ . \tag{3}$$

We work in the $P = 0$, parity even, $\mathbb{Z}_2$ even subsector of the truncated Hilbert space.
The interaction is

$$V = g\int_0^L dx \ :\phi^4(x): \ . \tag{4}$$

Expand V in bosonic creation and annihilation operators to compute its matrix elements.

Basis States

Quantise the massive scalar field on the circle

$$\phi(x) = \sum_{n=-\infty}^{\infty} \frac{1}{\sqrt{2LE_n}} \left(a_n \, e^{ik_n x} + a_n^\dagger \, e^{-ik_n x} \right) \ . \tag{5}$$

where the n represent the different momentum modes on the circle $k_n = 2\pi n/L$.

Work in eigenbasis of H_0

$$|\{\mathbf{r}\}\rangle = \prod_{n=-\infty}^{n=\infty} \frac{1}{\sqrt{r_n!}} \left(a_n^\dagger \right)^{r_n} |0\rangle \ , \tag{6}$$

which is the usual Fock basis.

Truncation

List the states in order of increasing H_0 eigenvalue and take the first 2^{n_q} states from this list.

For instance, with $n_q = 2$ and $mL = 3$, the states we would retain are

$$|0\rangle\,, \quad \frac{1}{\sqrt{2}}\left(a_0^\dagger\right)^2|0\rangle\,, \quad a_1^\dagger a_{-1}^\dagger|0\rangle\,, \quad \frac{1}{\sqrt{4!}}\left(a_0^\dagger\right)^4|0\rangle\,. \tag{7}$$

These states form our computational basis for quantum computing. Calculate matrix elements

$$V_{\mathbf{r},\mathbf{r}'} = \int dx \left\langle \{\mathbf{r}'\}\right| : \phi^4(x) : |\{\mathbf{r}\}\rangle \tag{8}$$

between these states. Gives H as a $2^{n_q} \times 2^{nq}$ matrix

Pauli Decomposition

To do the calculation on a NISQ device, we decompose the Hamiltonian as

$$H = \sum_{i_1 \ldots i_{n_q}=0}^{3} \alpha_{i_1 \ldots i_{n_q}} \left(\sigma_{i_1} \otimes \cdots \otimes \sigma_{i_{n_q}} \right) \tag{9}$$

Any Hermitian matrix can be decomposed this way to yield real coefficients $\alpha_{i_1 \ldots i_{n_q}}$.

For a generic dense Hamiltonian matrix, there will be $\sim 4^{n_q}$ nonzero coefficients in this decomposition.

Trotterisation

We use the Trotter-Suzuki approximation to first order. Error $\sim O(t^2/n)$.

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle \approx \left[\prod_{i_1,\ldots,i_{nq}} e^{-i\frac{t}{n}\alpha_{i_1,\ldots,i_{nq}}\left(\sigma_{i_1}\otimes\cdots\otimes\sigma_{i_{nq}}\right)}\right]^n |\psi(0)\rangle \ . \quad (10)$$

The exponential of each Pauli term can be implemented on a qubit-based quantum device through a *short* sequence of single-qubit rotation gates and CNOT gates.

The number of gates needed per trotter step grows with the number of nonzero $\alpha_{i_1\ldots i_{nq}}$ coefficients. This is *exponential* growth.

JLP Algorithm

In the two papers [S. Jordan, K. Lee, J. Preskill '11], [JLP '11], an *efficient* quantum algorithm was presented for computing S-Matrix elements in massive ϕ^4 theory:

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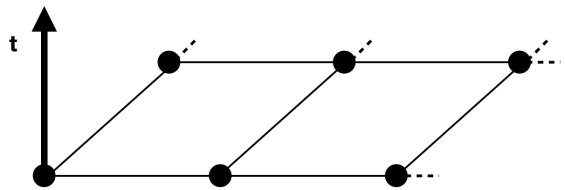

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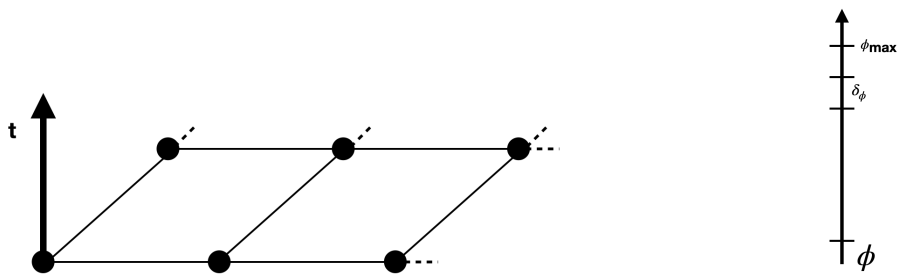

- The scalar field at each lattice site is also discretised. This is necessary to make the Hilbert space finite.

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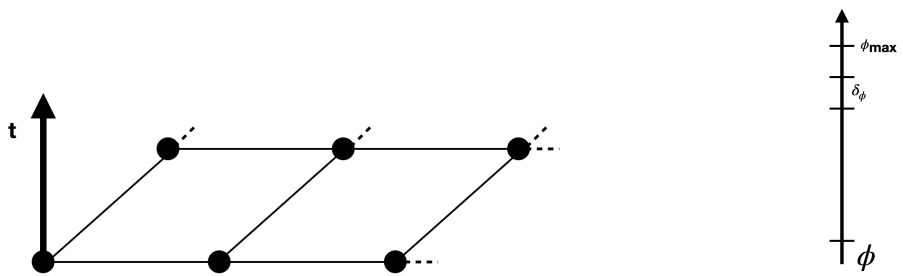
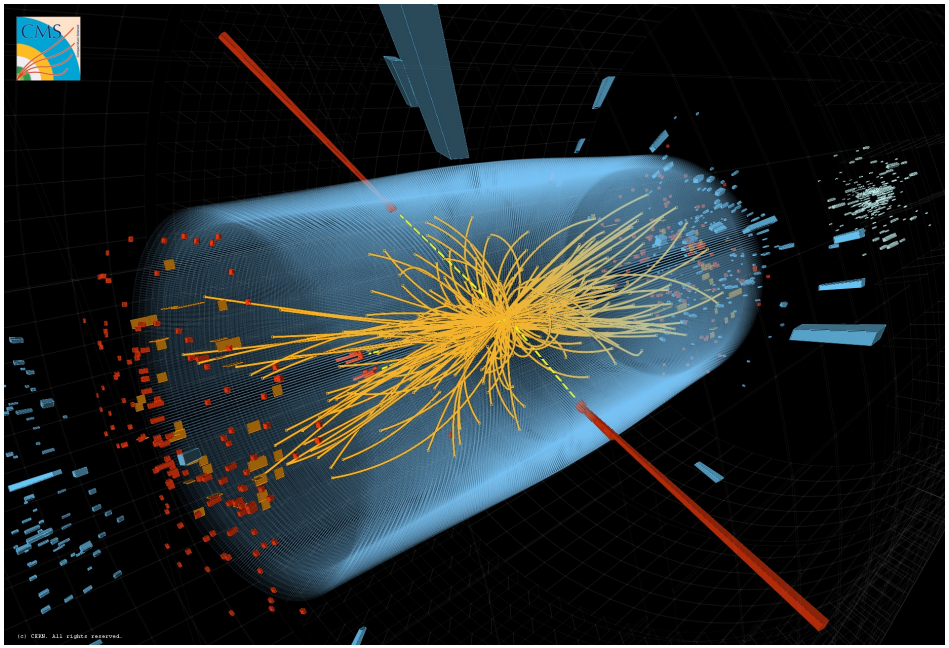


- The scalar field at each lattice site is also discretised. This is necessary to make the Hilbert space finite.
- Many followups e.g. [N. Zemlevskiy '24], [R. Konik et al '24].

Schematic Overview

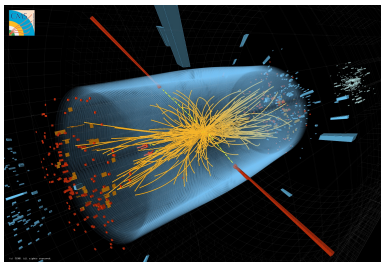
The JLP algorithm simulates a particle collision in real time.



It proceeds in 5 main steps...

The 5 Steps

1. Prepare vacuum of $\lambda = 0$ lattice theory [A. Kitaev, W. Webb '08].
2. Excite wavepackets of free theory.
3. Adiabatically switch on λ to get interacting theory wavepackets.
4. Time evolve until wavepackets collide and collision products separate.
5. Measure particle count in final state.



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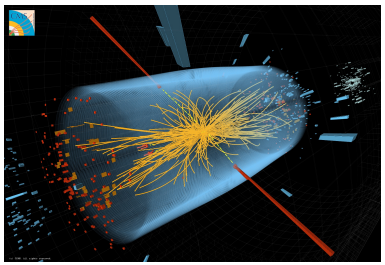

Comments:

- Quantum algorithm is exponentially faster than classical equivalents at high precision or strong coupling.
- Computes $2 \to n$ inelastic scattering. This is difficult for Euclidean space Lüscher method.

Generalising the JLP Algorithm to HT

What modifications are necessary in each of the 5 stages of the JLP algorithm?

1. Preparing the vacuum of the free theory $\Longrightarrow$ Automatic in HT

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3. Adiabatically switch on g to obtain interacting wavepackets $\implies$ We demonstrate for HT using quantum hardware.
4. Time evolve $\implies$ We demonstrate using classical simulators.
5. Measure particles in final state $\implies$ Straightforward in HT since computational basis is eigenbasis of particle number (in free theory).

Resource Costs

State of the art scattering simulations in ϕ^4 have been performed using 120 qubits on IBM hardware [N. Zemlevskiy '24].

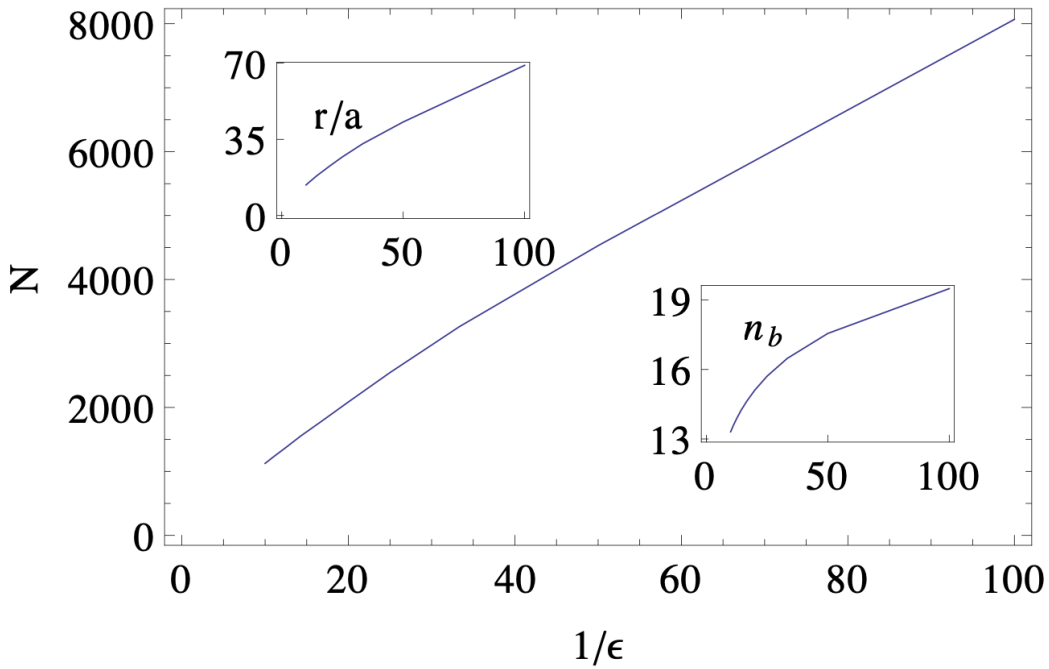


Figure: From [JLP '11] - number of qubits required to calculate $2 \to 4$ scattering amplitude in $1+1d$ with error ϵ. Interparticle separation is r/a.

Qubit Resources in HT

To simulate a collision with energy $\sqrt{s}$, the max energy state in the truncated basis in HT E_{max}, or the lattice spacing should be

$$\sqrt{s} \ll E_{\text{max}} \approx 1/a$$

The number of qubits needed for lattice formulation:

$$N_q^{\text{lattice}} = n_b(L/a)$$

[N. Klco and M. Savage '18]

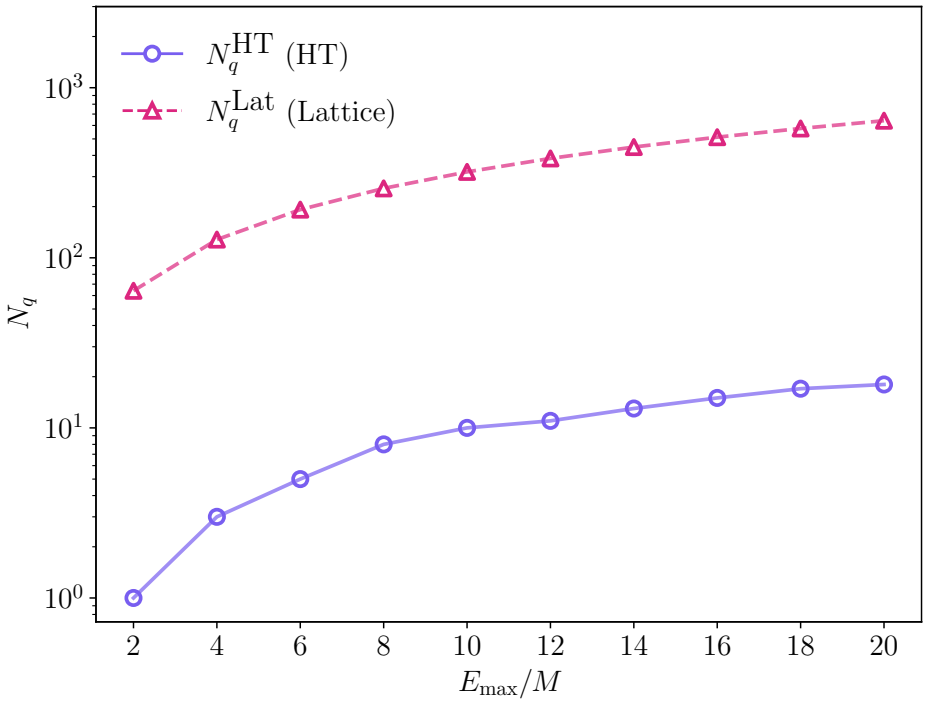


Figure: Comparing qubits needed for the lattice and HT formulations of scalar field theory, with $n_b = 2$, $ML = 16$.

Preparing Free Theory Wavepackets

Consider single particle Gaussian wavefunctions with $\langle x \rangle = x_0$, $\langle p \rangle = p_0$ and variance $\langle x^2 \rangle - \langle x \rangle^2 = \delta^2/2$:

$$\psi(x) = \mathcal{N} e^{-\frac{(x-x_0)^2}{2\delta^2}} e^{ip_0 x} \,. \tag{11}$$

We put this on the finite circle with little distortion provided that $\delta \ll L$, and that x_0 is far from the boundary.

A single particle state in the QFT can be built from the mom space wavefunction using

$$|\psi\rangle = \sum_{n=-\infty}^{\infty} \psi_{k_n} a_n^\dagger |0\rangle \,. \tag{12}$$

Projection Into Symmetry Subsector

Our initial state will be built from two well separated wavepackets at points $x_0 - L/4$ and $x_0 + L/4$, with opposite p_0:

$$|p_0, x_0, \delta\rangle = \mathcal{N} \sum_{\substack{n_1=-\infty \\ n_2=-\infty}}^{\infty} e^{i(k_{n_2}-k_{n_1})L/4} e^{-ix_0(k_{n_1}+k_{n_2})} \times$$

$$e^{-\frac{\delta^2}{2}\left[(p_0-k_{n_1})^2+(p_0+k_{n_2})^2\right]} a^\dagger_{n_1} a^\dagger_{n_2} |0\rangle \ . \quad (13)$$

In contrast to the lattice, it is natural in HT to simulate the scattering process in the zero momentum, parity even subsector of the QFT Hilbert space:

$$|p_0, \delta\rangle = \mathcal{N} \sum_{n=-\infty}^{\infty} (-1)^n e^{-\delta^2(p_0-k_n)^2} a^\dagger_n a^\dagger_{-n} |0\rangle \ . \quad (14)$$

Requirements for a Scattering State

- Wavepackets must be well separated with little overlap.
- Wavepacket group velocity $v_g \approx p_0/E_0$ should be bigger than broadening rate $\dot{\delta} \approx 1/(E_0\delta)$.

Consistency Condition

$$1/p_0 \ll \delta \ll L \tag{15}$$

Efficient Preparation on Quantum Hardware

Initial State

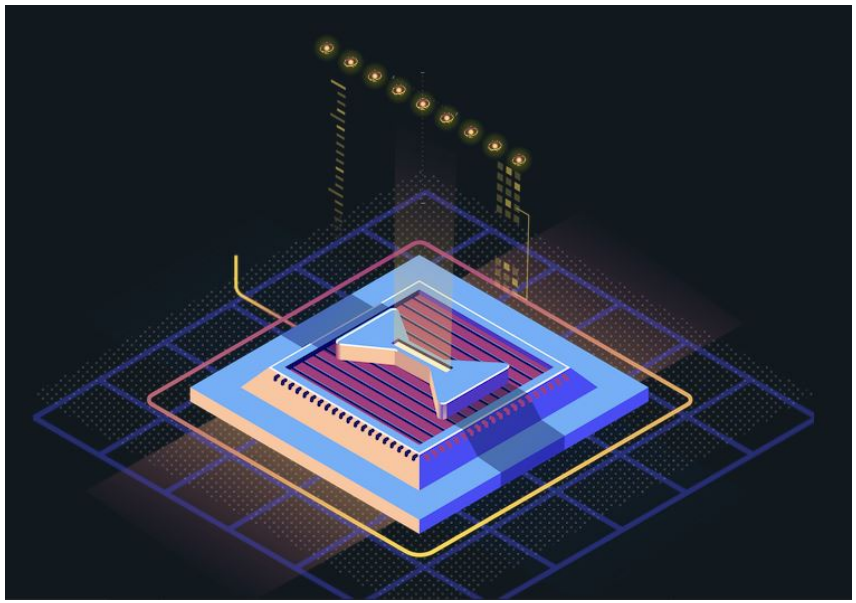
$$|p_0, \delta\rangle = \mathcal{N}' \Bigg(\sum_{n=1}^{N_{\max}} (-1)^n \left[e^{-\delta^2 (p_0 - k_n)^2} + e^{-\delta^2 (p_0 + k_n)^2} \right] |n, -n\rangle + \sqrt{2} e^{-\delta^2 p_0^2} |0, 0\rangle \Bigg), \quad (16)$$

- Retaining only $N_{\max}$ terms introduces only exponentially small error.
- States can be reordered within the truncated basis so that the two-particle states in Eq. (16) come first in the list.
- Represent on a subset of the qubits of length $n_q^{\text{sub}} = \lceil \log_2(N_{\max} + 1) \rceil$.
- Use quantum Shannon decomposition.

Trapped Ions

We use the "aria-1" device from IonQ, with 25 qubits.

- Qubits are Yb-171$^+$ ions.
- Longer coherence times and higher 2Q gate fidelity.
- All to all connectivity.
- Gate operations must be applied in series (rather than parallel).



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Free Theory State Preparation

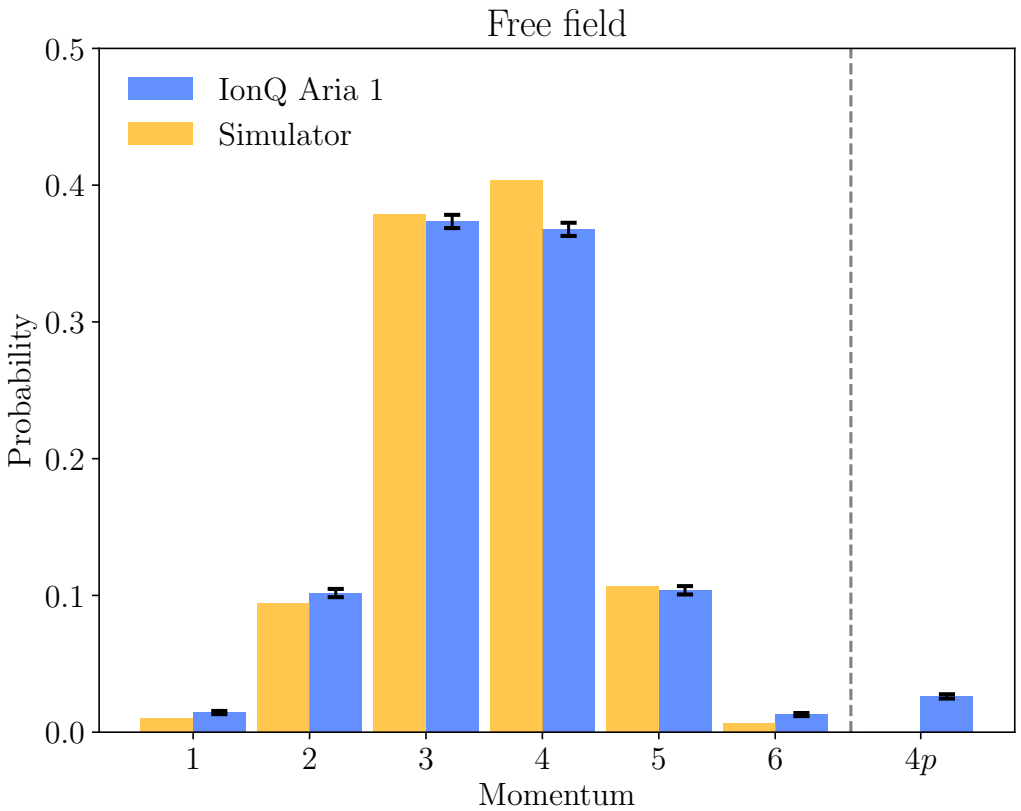


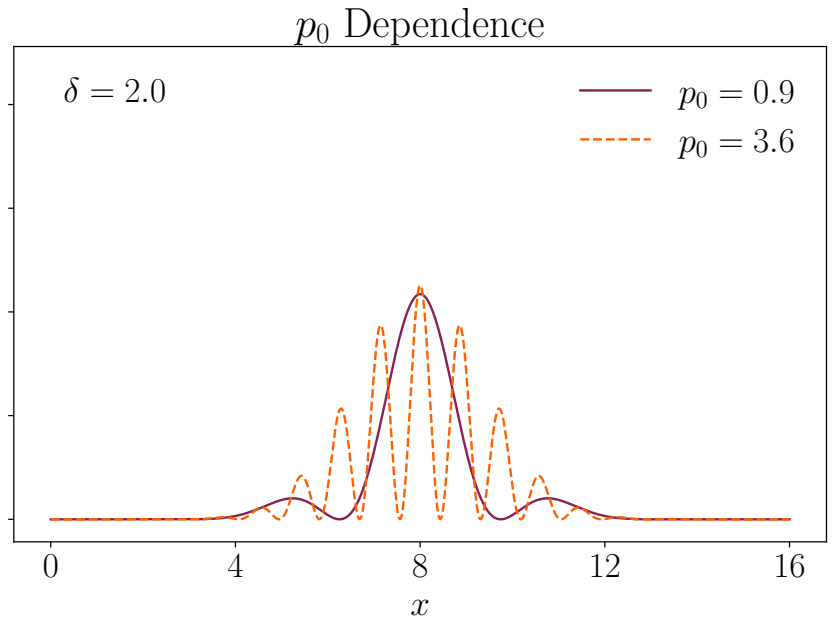
Figure: Probability of free wavepacket being measured in different H_0 eigenstates. Basis was truncated so that $n_q = 4$, but only $n_q^{\text{sub}} = 3$ were manipulated. Parameters: $ML = 16$, $p_0/M = 1.5$, $M\delta = 0.75$. Circuit has 13 gates.

Spatial Profile of the Wavepackets

The centre of mass is completely undetermined, but the separation between particles in the 2-particle sector is not:

$$\rho(x_1, x_2) = |x_1,\, x_2\rangle \langle x_1,\, x_2| \,\big|_{\mathbb{P},\, P}\,. \tag{17}$$

- Depends only on $x \equiv |x_1 - x_2|$.
- Has periodicity $x \to x + L$.
- Interference between terms with separations $\pm L/2$. Packets are not interacting as $\rho(x)$ is a nonlocal operator.



Interacting Theory Wavepackets

Adiabatically increase the ϕ^4 coupling g.
Incrementally increase g with each trotter step of time evolution.
Although free wavepackets are not energy eigenstates, a well separated packet that is concentrated in momentum space is approximately an eigenstate.
Avoid the Ising CFT critical point: $g(t) < g_c \sim 2.5 - 3$ (e.g. [S. Rychkov, L. Vitale '14])
(Optionally) evolve back in time after every few Trotter steps to reduce packet displacement and broadening.
Adiabatic time [JLP '11]

$$\tau \sim \frac{J}{\gamma^2 \sqrt{\epsilon}}$$

Interacting Theory State Preparation

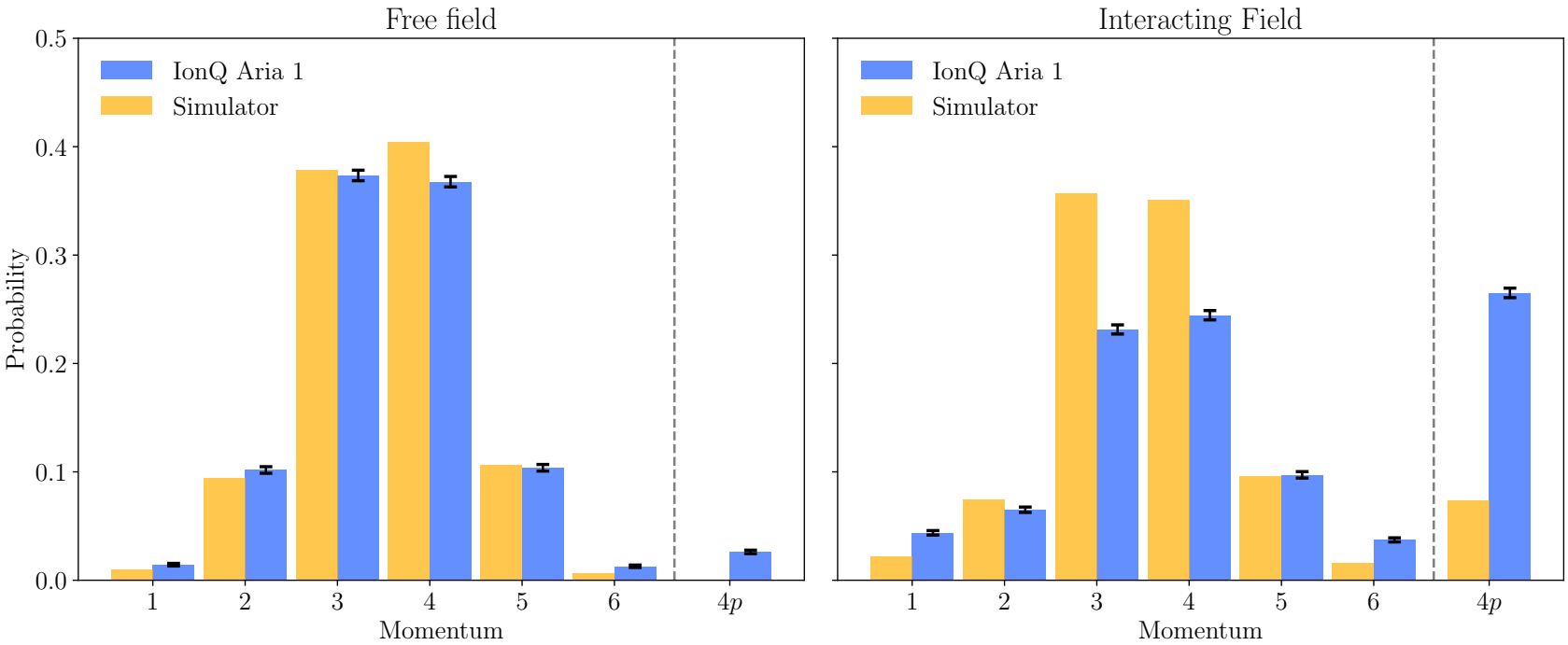


Figure: Right panel shows probability of interacting wavepacket being measured in different H_0 eigenstates. Basis was truncated so that $n_q = 4$. Parameters: $g = 2M^2$, $ML = 16$, $p_0/M = 1.5$, $M\delta = 0.75$. Circuit has 134 gates. Left panel shows free theory for comparison.

Time Evolution Of Wavepackets

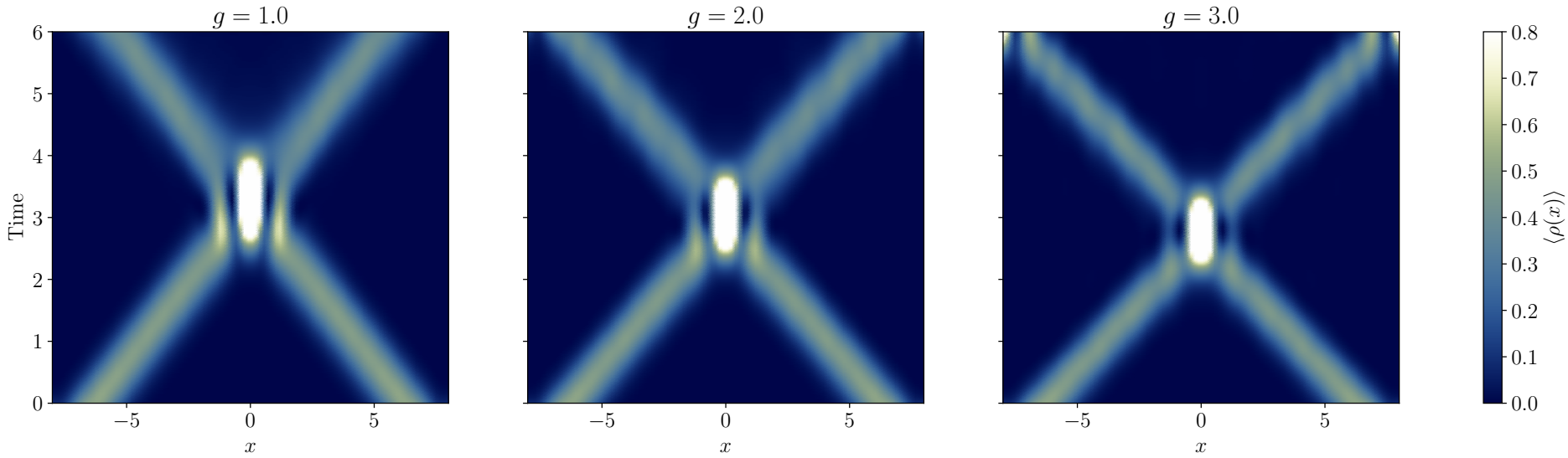


Figure: Classical computation of $\langle\rho(x)\rangle$ in the interacting theory using $n_q = 10$. We have taken $g = 2M^2$, $p_0/M = 2.5$, $M\delta = 0.75$, a displacement of $Mt = 1.5$, a Trotter step of $M\delta t = 0.01$ and a ramp time $M\tau = 1$. Note that we have not performed any extrapolation in E_{max}.

4 Particle Production Cross Section

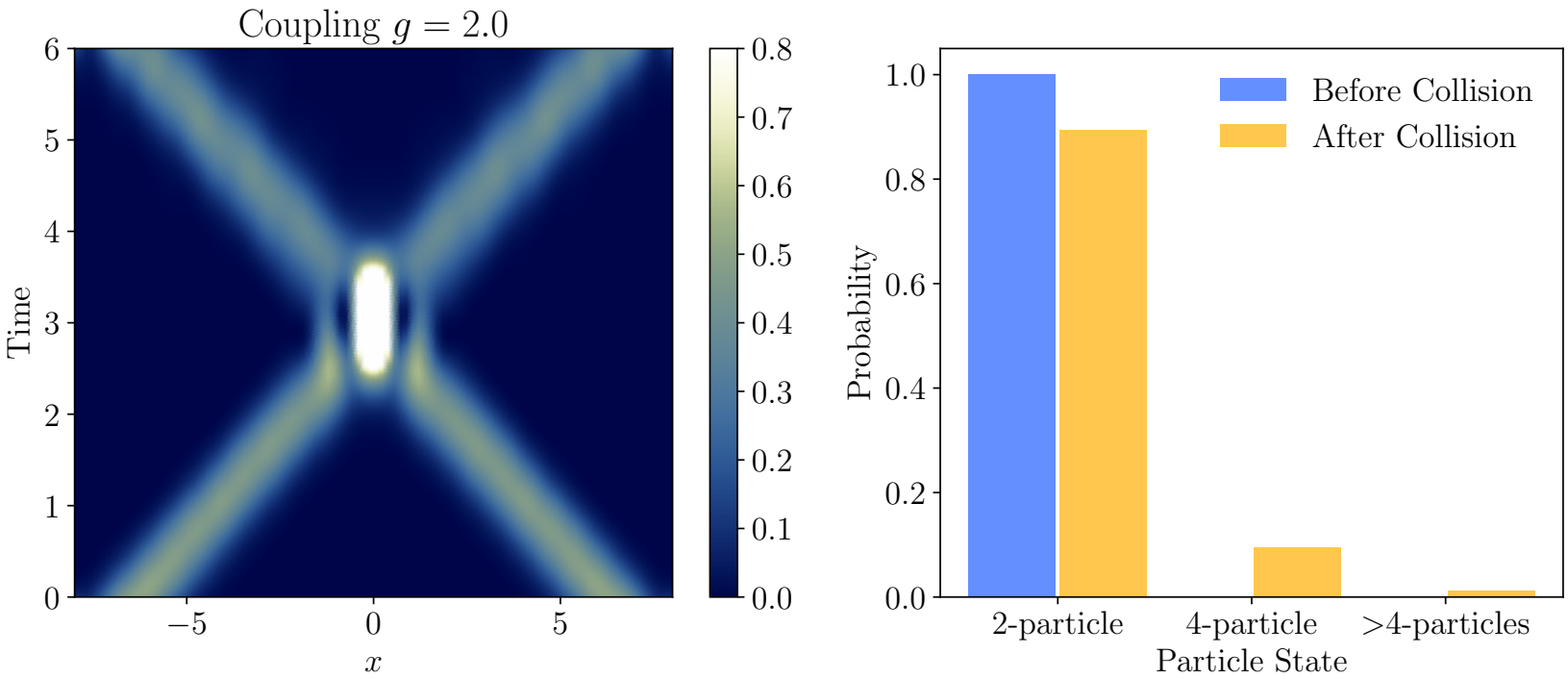


Figure: Scattering driven particle production. We have used $n_q = 10$, $g = 2M^2$, $p_0/M = 2.5$, $M\delta = 0.75$, a displacement of $Mt = 1.5$, a Trotter step of $M\delta t = 0.01$ and a ramp time $M\tau = 1$. This is just a proof of principle: No extrapolation has been attempted in E_{max} or in other simulation parameters.

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- We presented nonperturbative HT formulations for ϕ^4 theory.
- Near term progress in quantum computing will dramatically extend the reach of the HT approach.
- HT requires fewer qubits than other approaches to quantum simulation.
- We demonstrated quantum algorithms for time evolution and state preparation on a NISQ era trapped ion quantum device.

Thank you!

IBM Brisbane

Viewed on March 20th at 17:16 GMT from https://quantum.ibm.com/services/resources

ibm_brisbane Pulse gates

Details

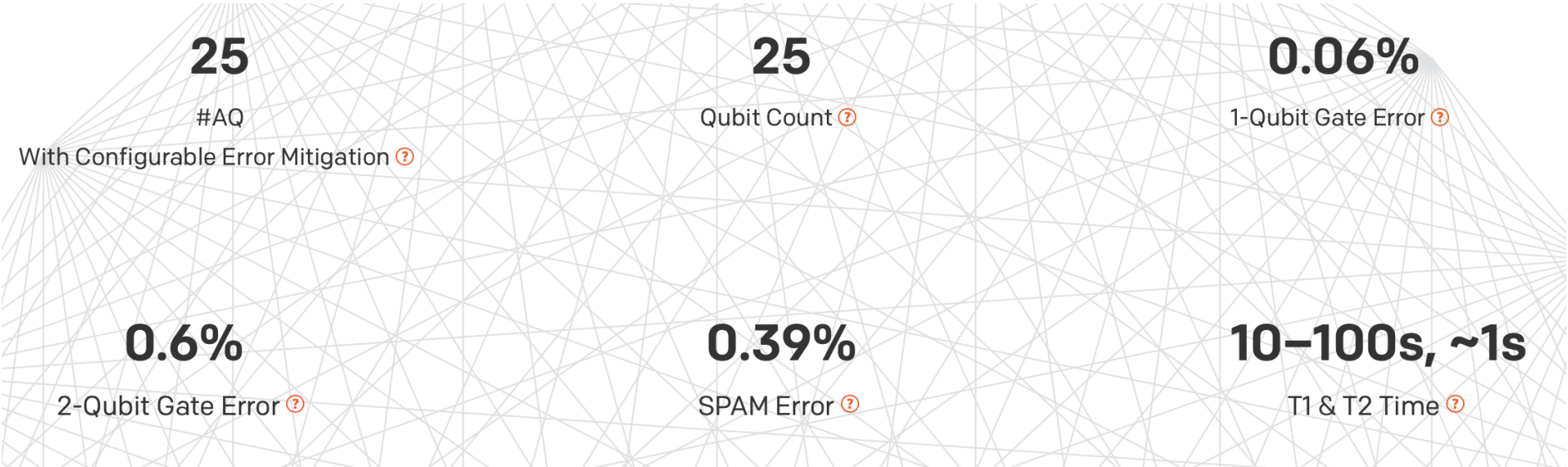
Qubits	2Q error (best)	2Q error (layered)	CLOPS
127	3.28e-3	1.69e-2	180K

Status:	Region:	Processor type ⓘ:	Version:
Online	us-east	Eagle r3	1.1.85

Total pending workloads:	Basis gates:	Median ECR error:	Median SX error:
12 jobs	ECR, ID, RZ, SX, X	7.519e-3	2.236e-4

Median readout error:	Median T1:	Median T2:
1.660e-2	230.85 us	154.59 us

Ionq Aria


25
#AQ
With Configurable Error Mitigation
25
Qubit Count
0.06%
1-Qubit Gate Error
0.6%
2-Qubit Gate Error
0.39%
SPAM Error
10–100s, ~1s
T1 & T2 Time

HT and Hamiltonian Lattice Generalities

HT Prioritises Symmetry

- Available when QFT has no known lattice formulation (e.g. exotic CFT with relevant deformations).
- Exact spacetime symmetries: Translations, Rotations and downstream: Chiral Symmetries, SUSY...
- Easier to impose conservation laws by removing entire sectors from Hilbert space $\implies$ fewer qubits.

HT and Hamiltonian Lattice Generalities

HT Deprioritises Locality

- Nonlocal counterterms sometimes necessary for renormalisation.
- Hamiltonian includes almost all-to-all interactions between the different qubits. Not the case for lattice Hamiltonians since qubits representing distant lattice sites do not interact.
- Leads to a dense representation in terms of Pauli strings, poor circuit depth scaling for time evolution using Suzuki-Trotter approach.

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- Difficulty also encountered when simulating other quantum systems that lack manifest locality, e.g. Matrix Models [M. Hanada et al '20].
- Discussed in lightcone truncation context: [J. Liu , Y. Xin '20], [M. Kreshchuk et al '20].

Sparsity and Qubitization

For time evolution with *sparse* Hamiltonians, shallower circuits can be found using post-trotter methods.

H enters the algorithm through "oracles", black boxes which give the position and value of nonzero matrix elements. [D. Berry, A. Childs '15]

Efficient Simulation

$$\text{queries} = \mathcal{O}\left(\tau \frac{\log(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right), \tag{18}$$

$$2 \text{ qubit gates} = \mathcal{O}\left(\tau n_q \frac{\log^2(\tau/\epsilon)}{\log\log(\tau/\epsilon)}\right). \tag{19}$$

Sparsity - d is max number of nonzero entries in any row of H.
Time - $\tau \equiv d^2 ||H||_{\max} t$.

Sparsity in HT ϕ^4 Theory

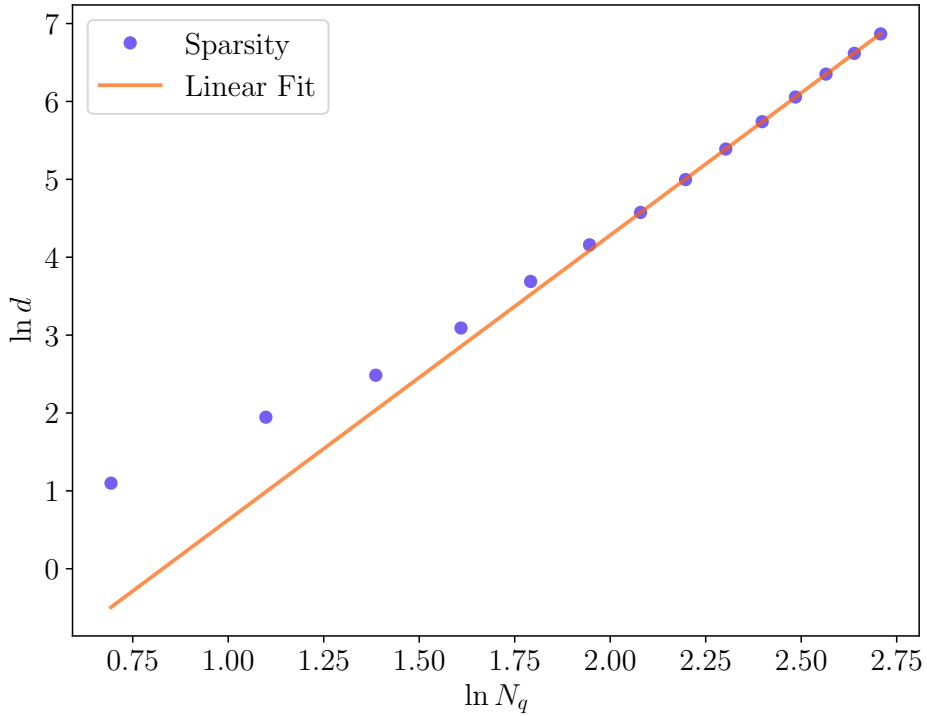

Figure: Log-Log plot showing the growth in the number of nonzero matrix elements in the truncated HT Hamiltonian with qubit number N_q. We find $d \ll 2^{N_q}$ throughout, indicating the Hamiltonian is sparse. The linear fit has the form $\ln d = 3.6651(63) \ln N_q - 3.028(15)$.