

Simulating ion trap quantum computers

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Shaw A. Simulating ion trap quantum computers. J Mod Appl Phys. 2022; 6(2):1-20.

ABSTRACT

An ion trap quantum computer is simulated with an exponential speed-up using the Stroboscopic Exponentiation Algorithm (SEA). It

leverages Hamiltonian periodicity for time-efficient quantum-simulation

Key Words: Quantum Simulation, Ion Trapping, Quantum, Error Correction

1. INTRODUCTION

Richard Feynman postulated the principle of quantum supremacy: quantum computers possess an innate computing advantage over classical computers [1].

Ion Trap Quantum Computing

Ion trap quantum computers (Figure 1) were proposed by Ignacio Cirac and Peter Zoller in May 1995 [2]. Ion trap quantum computers were experimentally demonstrated by Christopher Monroe et al. in December 1995 [3]. Ion trap quantum computers are the primary market competitors for transmon quantum computers [4–6].

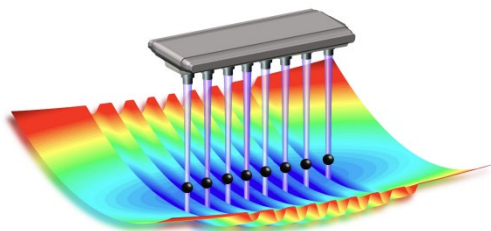


Figure 1) An ion trap quantum computer is composed of ions (black) confined using electromagnetic fields (rainbow). The electronic states are manipulated using lasers (purple)

Ion Trapping

An ion trap confines charged atoms to a spatial region using time-dependent electromagnetic fields [7–18].

Quantum operations

Atomic qubits are pairs of electronic states associated with each ion (Figure 2) [19]. Lasers can induce transitions between the electronic states [20–29].

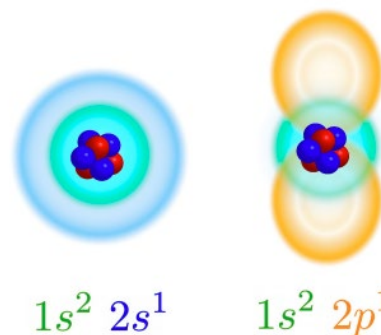


Figure 2) An atomic qubit is composed of a spin-down (left) and spin-up (right) electronic state

2. ION TRAP QUANTUM COMPUTERS

The Hamiltonian for an ion trap quantum computer is derived from quantum theory [30,31].

1. Ion Trap Hamiltonian

Ionic Hamiltonian

The ion trap parameters are the following:

$$\text{Atomic Number: } Z \quad (2.1)$$

$$\text{Ion Charge: } Q_e \quad (2.2)$$

$$\text{Ion Mass: } M \quad (2.3)$$

$$\text{Number of Ions: } N \quad (2.4)$$

a) Kinetic Interactions: The ionic kinetic energy operator is the following [32]:

$$\hat{K}_{ion} = -\frac{1}{2M} \sum_{i=1}^N \vec{\nabla}_i^2 \quad (2.5)$$

b) Ionic Interactions: The ionic electrostatic operator is the following [33]:

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Received:- 20 Feb, 2023, Manuscript No. puljmap-23-6151; Editor assigned:- 22 Feb, 2023, Pre-QC No. puljmap-23-6151 (PQ); Reviewed:- 27 Feb, 2023, QC No. puljmap-23-6151 (Q); Revised:- 7 Mar, 2023, Manuscript No. puljmap-23-6151 (R); Published:- 23 Mar 2023, DOI: 10.37532.2022.6.1.1-20



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$$\hat{V}_{elec}^{(ion)} = \frac{(Qe)^2}{8\pi} \sum_{\substack{i,j=1 \\ i \neq j}}^N \frac{1}{\left| \vec{x}_i - \vec{x}_j \right|} \quad (2.6)$$

c) Trapping potential: The trap electric field is the following [8]:

$$\vec{E}_{trap}(\vec{x}, t) = \vec{E}_{static}(\vec{x}) + \vec{E}_{dynamic}(\vec{x}) \cos(\Omega_r t) \quad (2.7)$$

The trap scalar potential is the following [34]:

$$\phi_{trap}(\vec{x}, t) \approx - \int_{x_r}^{\vec{x}} \vec{E}_{trap}(\vec{x}', t) \times d\vec{l}' \quad (2.8)$$

The trapping operator is the following:

$$\hat{V}_{trap}(t) = Qe \sum_{i=1}^N \hat{\phi}_{trap}(\vec{x}_i, t) \quad (2.9)$$

Over a timescale $t_{trap} \ll 2\pi/\Omega_r$, the trapping operator can be approximated by a confining operator [35–37]:

$$\hat{V}_{trap}(t) \approx \hat{V}_{confiner} \quad (2.10)$$

d) Ion-laser interaction: The laser electric field is the following:

$$\vec{E}_{laser}(\vec{x}, t) = \vec{E}_0(\vec{x}) e^{i(\vec{k} \cdot \vec{x} - \omega t)} \quad (2.11)$$

The laser magnetic vector potential is given by the following [38]:

$$\vec{\nabla}^2 \vec{A}_{laser}(\vec{x}, t) = - \frac{\partial \vec{E}_{laser}(\vec{x}, t)}{\partial t} \quad (2.12)$$

The laser magnetic field is the following:

$$\vec{B}_{laser}(\vec{x}, t) = \vec{\nabla} \times \vec{A}_{laser}(\vec{x}, t) \quad (2.13)$$

The laser scalar potential is the following:

$$\phi_{laser}(\vec{x}, t) = - \int_{x_r}^{\vec{x}} \left[E_{laser}(\vec{x}', t) + \frac{\partial \vec{A}_{laser}(\vec{x}', t)}{\partial t} \right] \cdot d\vec{l}' \quad (2.14)$$

The ionic laser operator is the following:

$$\begin{aligned} \hat{V}_{laser}^{(ion)}(t) &= \sum_{i=1}^N \frac{iQe}{2M} \left(\hat{A}_{laser}(\vec{x}_i, t) + \hbar \cdot \vec{c} \right) \times \vec{\nabla}_i \\ &+ \frac{(Qe)^2}{8M} \left(\vec{A}_{laser}(\vec{x}_i, t) + \hbar \cdot \vec{c} \right)^2 \\ &+ \frac{Qe}{2} (\hat{\phi}_{laser}(\vec{x}_i, t) + \hbar \cdot \vec{c}) \end{aligned} \quad (2.15)$$

e) Ionic Hamiltonian: The ionic Hamiltonian is the following:

$$\hat{H}_{ion}(t) = \hat{K}_{ion} + \hat{V}_{elec}^{(ion)} + \hat{V}_{confiner} + \hat{V}_{laser}^{(ion)}(t) \quad (2.16)$$

2. Electronic Hamiltonian

a) Electron number: The number of electrons in the trap is the following:

$$N_e = N(Z - Q) \quad (2.17)$$

b) Kinetic Term: The electronic kinetic energy operator is the following:

$$\hat{K}_e = - \frac{1}{2m_e} \sum_{r=1}^{N_e} \vec{\nabla}_r^2 \quad (2.18)$$

c) Atomic well: The atomic well operator is the following:

$$\hat{V}_{atom} = - \frac{Z_e^2}{4\pi} \sum_{i=1}^N \sum_{\substack{r=1 \\ r \neq s}}^{N_e} \frac{1}{\left| \vec{x}_i - \vec{y}_r \right|} \quad (2.19)$$

d) Electronic interactions: The electronic electrostatic operator is the following:

$$\hat{V}_{elec}^{(e)} = - \frac{e^2}{8\pi} \sum_{\substack{r,s=1 \\ r \neq s}}^{N_e} \frac{1}{\left| \vec{y}_r - \vec{y}_s \right|} \quad (2.20)$$

e) Electron-laser interactions: The electronic laser operator is the following [39]:

$$\begin{aligned} \hat{V}_{laser}^{(e)}(t) &= \sum_{r=1}^{N_e} \frac{e}{2im_e} (\hat{A}_{laser}(\vec{y}_r, t) + \hbar \cdot \vec{c}) \cdot \vec{\nabla}_r \\ &+ \frac{e^2}{8m_e} \left(\vec{A}_{laser}(\vec{y}_r, t) + \hbar \cdot \vec{c} \right)^2 + \frac{e}{4m_e} \vec{\sigma}_r^{(s)} \times \left(\vec{B}_{laser}(\vec{y}_r, t) + \hbar \cdot \vec{c} \right) \\ &- \frac{e}{2} (\hat{\phi}_{laser}(\vec{y}_r, t) + \hbar \cdot \vec{c}) \end{aligned}$$

f) Electronic Hamiltonian: The electronic Hamiltonian is the following:

$$\hat{H}_{electron}(t) = \hat{K}_e + \hat{V}_{atom} + \hat{V}_{elec}^{(e)} + \hat{V}_{laser}^{(e)}(t) \quad (2.21)$$

3. Qubit Hamiltonian

a) Qubit States: The atomic orbital Hamiltonian for a single ion at \vec{x} is the following [40]:

$$\hat{H}_{orbital}^{(\vec{x})} = \sum_{r=1}^{N_e/N} \frac{\vec{p}_r^2}{2m_e} - \frac{Ze^2}{4\pi \left| \vec{x} - \vec{y}_r \right|} \quad (2.22)$$

The atomic orbital Hamiltonian's eigenstates form a complete basis centered at \vec{x} :

$$\hat{H}_{orbital}^{(\vec{x})} |\alpha_{orbital}(\vec{x})\rangle = \lambda_{\alpha}^{(\vec{x})} |\alpha_{orbital}(\vec{x})\rangle \quad (2.23)$$

The qubit states are the following (Figure 2):

$$|\psi_q^{(\uparrow)}(\vec{x})\rangle = \sum_{\alpha} c_{\alpha}^{(\uparrow)} |\alpha_{orbital}(\vec{x})\rangle \quad (2.24)$$

$$|\psi_q^{(\downarrow)}(\vec{x})\rangle = \sum_{\alpha} c_{\alpha}^{(\downarrow)} |\alpha_{orbital}(\vec{x})\rangle \quad (2.25)$$

b) Passenger-Qubit Hilbert Space: The passenger-qubit Hilbert space at \vec{x} is spanned by two states:

$$H_q(\vec{x}) = \text{span}\{|\vec{x}\rangle \otimes |\psi_q^{(\uparrow)}(\vec{x})\rangle, |\vec{x}\rangle \otimes |\psi_q^{(\downarrow)}(\vec{x})\rangle\} \quad (2.26)$$

In the passenger-qubit construction, the qubit states co-move with the ion (Figure 3).

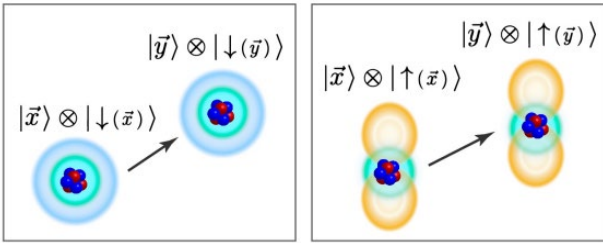


Figure 3 The spin-down (left panel) and spin-up (right panel) qubit states vary with the ion position

c) Passenger-Qubit Basis States: In the multi-ion case, the passenger-qubit basis states are the following:

$$|\{\vec{x}\}, \vec{\alpha}\rangle = |\vec{x}_1\rangle |\vec{x}_2\rangle \dots |\vec{x}_N\rangle \otimes |\psi_q^{(\alpha_1)}(\vec{x}_1)\rangle |\psi_q^{(\alpha_2)}(\vec{x}_2)\rangle \dots |\psi_q^{(\alpha_N)}(\vec{x}_N)\rangle \quad (2.27)$$

d) Qubit Operators: Qubit operators are projections of the electronic Hamiltonian into the passenger-qubit Hilbert space. To avoid an adiabatic effective Hamiltonian description, a passenger-qubit Hilbert space is required for hyperfine qubits [41-43].

$$\hat{p}(\{\vec{x}_i\}, t) = \sum_{\vec{\alpha}, \vec{\beta}} \langle \{\vec{x}_i\}, \vec{\alpha} | \hat{H}_{electron}(t) | \{\vec{x}_i\}, \vec{\beta} \rangle$$

$$| \{\vec{x}_i\}, \vec{\alpha} \rangle \langle \{\vec{x}_i\}, \vec{\beta} | \quad (2.28)$$

e) Pauli Decomposition: The generalized Pauli operators are the following [44]:

$$\sum (\vec{p}) = \hat{\sigma}_{p_1} \otimes \sigma_{p_2} \otimes \dots \sigma_{p_N} \quad (2.29)$$

$$p_i \in \{0, 1, 2, 3\} \quad (2.30)$$

The qubit operators are decomposed in the generalized Pauli basis [45]:

$$\hat{p}(\{\vec{x}_i\}, t) = \sum_{\vec{p}} \kappa(\vec{p}, t) \hat{\sum}(\vec{p}) \quad (2.31)$$

f) Qubit Hamiltonian: The qubit Hamiltonian is the following:

$$\hat{H}_{qubit}(t) = \left(\prod_{i=1}^N \int d^3x_i \right) \hat{p}(\{\vec{x}_i\}, t) \quad (2.32)$$

4. Ion Trap Hamiltonian

The ion trap Hamiltonian is the following:

$$\hat{H}_{ion trap}(t) = \hat{H}_{ion}(t) + \hat{H}_{qubit}(t) \quad (2.33)$$

2. Vibrational Expansion

The vibrational expansion approximates the near equilibrium ion trap dynamics by collective oscillatory motion [46].

1. Vibrational Expansion

a) Total Ionic Potential Energy: In the absence of the laser, the ionic Hamiltonian is expressed using the total ionic potential energy operator:

$$\hat{H}_{ion} = \hat{K}_{ion} + \hat{V}_{elec}^{(ion)} + \hat{V}_{confine} \quad (2.34)$$

$$= \hat{K}_{ion} + \hat{V}_{total} \quad (2.35)$$

b) Ionic Component Vector: The ionic position components are the following:

$$\vec{x}_i = \{x_i^{(1)}, x_i^{(2)}, x_i^{(3)}\} \quad (2.36)$$

They are used to form the ionic component vector:

$$\vec{c} = \{x_1^{(1)}, x_1^{(2)}, x_1^{(3)}; x_2^{(1)}, x_2^{(2)}, x_2^{(3)}; \dots; x_N^{(1)}, x_N^{(2)}, x_N^{(3)}\} \quad (2.37)$$

c) Component Gradient: The component gradient is the gradient with respect to the ionic component vector:

$$\vec{\nabla}_{comp} = \sum_{k=1}^{3N} c_k \frac{\partial}{\partial c_k} \quad (2.38)$$

d) Critical Point: A critical point of the total ionic potential energy occurs at \vec{c}_0 :

$$\vec{\nabla}_{comp} \nabla_{total}(\vec{c})|_{\vec{c}=\vec{c}_0} = \vec{0} \quad (2.39)$$

The vibrational expansion is made by expanding the total ionic potential energy around \vec{c}_0 :

$$V_{total}(\vec{c}) = \sum_{n=0}^{\infty} \frac{1}{n!} (\vec{\nabla}_{comp})_{\otimes_{outer}}^n V_{total}(\vec{c})|_{\vec{c}=\vec{c}_0} \times (\vec{c} - \vec{c}_0)_{\otimes_{outer}}^n \quad (2.40)$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} (\vec{\nabla}_{comp})_{\otimes_{outer}}^n V_{total}(\vec{c})|_{\vec{c}=\vec{c}_0} \times (\vec{\nabla}_c)^n_{\otimes_{outer}} \quad (2.41)$$

$$= \sum_{n=0}^{\infty} v_n(\vec{c}) \quad (2.42)$$

e) Potential Hessian Matrix: The second-order contribution to the vibrational expansion is expressed as a matrix equation:

$$v_2(\vec{c}) = (\Delta_c)^T \hat{A}(\Delta_c) \quad (2.43)$$

$$= \sum_{m,n=1}^{3N} (\Delta c)_m \hat{A}_{m,n} (\Delta c)_n \quad (2.44)$$

The potential Hessian matrix is the following [9]:

$$\hat{A}_{a,b} = \frac{1}{2} \frac{\partial}{\partial c_a} \frac{\partial}{\partial c_b} V_{total}(\vec{c}) \Big|_{\vec{c}=\vec{c}_0} \quad (2.45)$$

f) Trap Frequencies: The potential Hessian matrix is diagonalized as follows:

$$\hat{A} = \hat{O}^T \hat{D} \hat{O} \quad (2.46)$$

The eigenvalues of the potential Hessian matrix provide access to the trap frequencies:

$$\hat{D}_{a,a} = \omega_a^2 \quad (2.47)$$

2. Ladder Hamiltonian

a) Vibrational Mode Vector: The vibrational mode vector is the following (Figure 4):

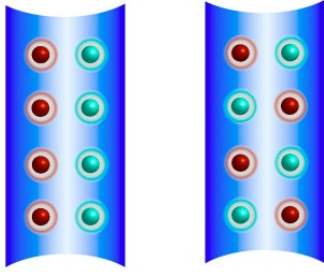


Figure 4) The ions oscillate collectively (red \longleftrightarrow green) in the ion trap (blue). The center-of-mass mode (left) and the zig-zag mode (right) are shown [42].

$$\vec{m} = \hat{O} \vec{\Delta}_c \quad (2.48)$$

$$m_a = \sum_{b=1}^{3N} \hat{O}_{a,b} (c_b - c_{0,b}) \quad (2.49)$$

b) Harmonic Interactions: The second-order contribution to the vibrational expansion is written in harmonic form:

$$\nu_2(\vec{c}) = (\vec{\Delta}_c)^T \hat{O}^T \hat{D} \hat{O} (\vec{\Delta}_c) \quad (2.50)$$

$$= (\vec{m})^T \hat{D} (\vec{m}) \quad (2.51)$$

$$= \sum_{a=1}^{3N} \omega_a^2 m_a^2 \quad (2.52)$$

c) Component Laplacian: The component Laplacian is the following:

$$\vec{\nabla}_{comp}^2 = \sum_{k=1}^{3N} \frac{\partial^2}{\partial c_k^2} \quad (2.53)$$

The first partial derivative is expressed in terms of the vibrational mode vector components (Equation 2.49):

$$\frac{\partial}{\partial c_k} = \sum_{a=1}^{3N} \frac{\partial m_a}{\partial c_k} \frac{\partial}{\partial m_a} \quad (2.54)$$

$$= \sum_{a=1}^{3N} \hat{O}_{a,k} \frac{\partial}{\partial m_a} \quad (2.55)$$

The component Laplacian is the following:

$$\vec{\nabla}_{comp}^2 = \sum_{k=1}^{3N} \sum_{a,b=1}^{3N} (\hat{O}_{a,k})(\hat{O}_{b,k}) \left(\frac{\partial^2}{\partial m_a \partial m_b} \right) \quad (2.56)$$

$$= \sum_{a,b=1}^{3N} \delta_{a,b} \frac{\partial^2}{\partial m_a \partial m_b} = \sum_{k=1}^{3N} \frac{\partial^2}{\partial m_a^2} \quad (2.57)$$

d) Kinetic Interactions: The ionic kinetic energy operator is the following:

$$\hat{K}_{ion} = -\frac{1}{2M} \sum_{k=1}^{3N} \frac{\partial^2}{\partial m_k^2} \quad (2.58)$$

$$= \frac{1}{2M} \sum_{k=1}^{3N} \hat{p}_k^2 \quad (2.59)$$

e) Ionic Hamiltonian: The ionic Hamiltonian is the following:

$$\vec{H}_{ion} = \sum_{k=1}^{3N} \frac{\hat{p}_k^2}{2M} + \omega_k^2 m_k^2 + o(|\vec{\Delta}_c|^3) \quad (2.60)$$

f) Mode Ladder Operators: The mode ladder operators are the following [47]:

$$\hat{a}_k^\dagger = \left(\frac{M \omega_k^2}{2} \right)^{\frac{1}{4}} \hat{m}_k - i \left(\frac{1}{8M \omega_k^2} \right)^{\frac{1}{4}} \hat{p}_k \quad (2.61)$$

$$\hat{a}_k = \left(\frac{M \omega_k^2}{2} \right)^{\frac{1}{4}} \hat{m}_k - i \left(\frac{1}{8M \omega_k^2} \right)^{\frac{1}{4}} \hat{p}_k \quad (2.62)$$

g) Ladder Hamiltonian: The ionic Hamiltonian becomes the following, up to an overall constant:

$$\vec{H}_{ion} = \sqrt{\frac{2}{M}} \sum_{k=1}^{3N} \omega_k \left\{ \hat{a}_k^\dagger \hat{a}_k \right\} + o(|\vec{\Delta}_c|^3) \quad (2.63)$$

The ionic Hamiltonian can be expressed in terms of the physical trap frequencies [48]:

$$\vec{H}_{ion} = \sum_{k=1}^{3N} \omega_k \left\{ \hat{a}_k^\dagger \hat{a}_k \right\} + o(|\vec{\Delta}_c|^3) \quad (2.64)$$

3. Effective Ion Trap Hamiltonian

Effective approximations are used to tailor the ion trap Hamiltonian for quantum computing applications [49].

1. Strong-Confinement Approximation

The Strong-Confinement Approximation (SCA) is the following (Figure 5):

$$\sum_{n=3}^{\infty} |\langle \hat{v}(n) \rangle| \ll |\langle \hat{v}(2) \rangle| \quad (2.65)$$

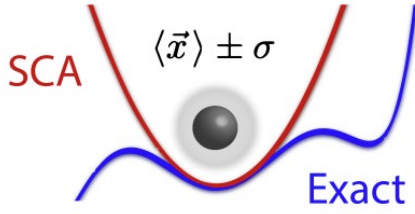


Figure 5) If the ion (gray) is strongly confined, the total potential energy (blue) can be approximated (red)

The effective ionic Hamiltonian is as follows:

$$\hat{H}_{ion}^{(eff)} = \sum_{k=1}^{3N} \omega_k \{ \hat{a}_k^\dagger \hat{a}_k \} \quad (2.66)$$

2. Weak-Laser Approximation

The Weak-Laser Approximation (WLA) is as follows (Figure 6):

$$|\langle \hat{V}_{laser}(t) \rangle| \ll |\langle \hat{H}_{ion} \rangle| \quad (2.67)$$

The effective ion trap Hamiltonian is the following:

$$\hat{H}_{ion trap}^{(eff)}(t) = \sum_{k=1}^{3N} \omega_k \{ \hat{a}_k^\dagger \hat{a}_k \} + \hat{H}_{qubit}(t) \quad (2.68)$$

$$= \hat{H}_{phonon} + \hat{H}_{qubit}(t) \quad (2.69)$$

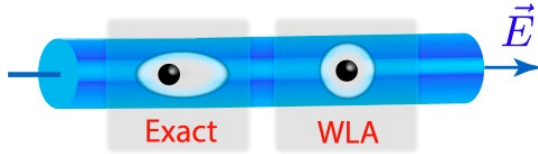


Figure 6) If the laser (blue) is sufficiently weak, its effect on the ionic wavefunction (left) can be neglected (right)

4. Interaction Picture Hamiltonian

1. Interaction Picture

The interaction picture leverages the effective ionic Hamiltonian's analytic evolution operator for faster computation [50].

a) Interaction Picture Hamiltonian: The effective interaction picture Hamiltonian is the following:

$$\hat{H}_{ion trap}^{(eff,I)}(t) = e^{it\hat{H}_{phonon}} \hat{H}_{qubit}(t) e^{-it\hat{H}_{phonon}} \quad (2.70)$$

2. Spin-Phonon Interactions

a) Phonon Passenger-Qubit Basis: The phonon passenger-qubit basis states are as follows:

$$\begin{aligned} |\vec{n}, \alpha\rangle &= |n_1\rangle |n_2\rangle \dots |n_{3N}\rangle \\ \otimes |\psi_q^{(\alpha_1)}(\vec{n})\rangle &|\psi_q^{(\alpha_2)}(\vec{n})\rangle \dots |\psi_q^{(\alpha_N)}(\vec{n})\rangle \end{aligned} \quad (2.71)$$

b) Spin-Phonon Operators: The spin-phonon operators are projections of the electronic Hamiltonian into the phonon passenger-qubit Hilbert space:

$$\hat{S}_{n \rightarrow m \alpha \beta}^{(t)} = |\vec{n}, \alpha\rangle \langle \vec{n}, \alpha| \hat{H}_{electron}(t) |\vec{m}, \beta\rangle \langle \vec{m}, \beta| \quad (2.72)$$

The effective interaction picture Hamiltonian is written explicitly:

$$\hat{H}_{ion trap}^{(eff,I)}(t) = \sum_{n \rightarrow m \alpha \beta} e^{it \sum_{k=1}^{3N} \omega_k (n_k - m_k)} \hat{S}_{n \rightarrow m \alpha \beta}^{(t)} \quad (2.73)$$

3. CLASSICAL QUANTUM-SIMULATION ALGORITHMS

An algorithm is proposed to efficiently simulate ion trap quantum computers.

A) Product-Formula Algorithms

Product-Formula Algorithms (PFAs) are a family of quantum-simulation algorithms [51, 52]. The PFA is an extremely versatile algorithmic framework, with mathematical, low-energy, and high-energy physics applications [53-82].

PFAs can be represented schematically in three stages:

1. Discretization: Subdivide the simulation time into sub-regions.
2. Piece-wise Simulation: Approximate the subregion evolution operators.
3. Matrix Multiplication: Take the ordered product of the sub-region evolution operators.

1. Evolution Operator

a) Hamiltonian Operator: The Hamiltonian is the following:

$$\hat{H}_{sim}(t) = \sum_{\alpha=1}^d \epsilon_{\alpha}(t) |\alpha(t)\rangle \langle \alpha(t)| \quad (3.1)$$

b) Time-Ordered Exponential

The evolution operator is the following:

$$\hat{U}_{sim}(t) = \tau \{ e^{-i \int_0^t dt' \hat{H}_{sim}(t')} \} \quad (3.2)$$

2. Discretization

a) Sub-Regions: The simulation time τ is subdivided into L_{sim} sub-regions:

$$\delta t = \frac{\tau}{L_{sim}} \quad (3.3)$$

b) Sub-Region Evolution Operators: The sub-region evolution operators are the following:

$$\hat{U}_{sub}^{(r)} = \tau \{ e^{-i \int_{(r-1)\delta t}^{r\delta t} dt' \hat{H}_{sim}(t')} \} \quad (3.4)$$

The evolution operator can be written as an ordered product of the sub-region evolution operators:

$$\hat{U}_{sim}(t) = \prod_{r=1}^{L_{sim}} \hat{U}_{sub}^{(r)} \quad (3.5)$$

$$= \hat{U}_{sub}^{(L_{sim})} \dots \hat{U}_{sub}^{(2)} \hat{U}_{sub}^{(1)} \quad (3.6)$$

c) Piece-Wise Simulation: An intermediate simulation algorithm is used to generate the approximate sub-region evolution operators:

$$\hat{U}_{\alpha,sub}^{(r)} = \hat{U}_{sub}^{(r)} + \mathcal{E}_{sub}^{(r)} \quad (3.7)$$

d) Matrix Multiplication: An ordered-product is used to generate the approximate evolution operator:

$$\hat{U}_{\alpha, sim}^{(r)}(t) = \prod_{r=1}^{L_{sim}} \hat{U}_{\alpha, sim}^{(r)} \quad (3.8)$$

B) Time-Integrated Product-Formula Algorithm

The Time-Integrated Product-Formula Algorithm (TI-PFA) coarse-grains the Hamiltonian to minimize the number of required sub-regions [83–85].

1. Time-Integrated Product-Formula Algorithm

TI-PFA can be represented schematically in three stages:

1. Time-Averaging: Time-average the Hamiltonian over the sub-regions.
2. Matrix Exponentiation: Generate the approximate sub-region evolution operators.
3. Matrix Multiplication: Take the ordered product of the approximate sub-region evolution operators.

a) Time-Averaging: The sub-region Hamiltonians are as follows (Figure 7):

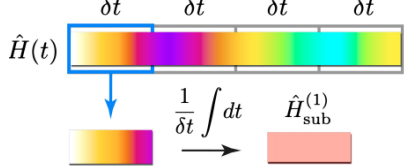
$$\hat{H}_{sub}^{(r)} = \frac{1}{\delta t} \int_{(r-1)\delta t}^{r\delta t} dt' \hat{H}_{sim}(t') \quad (3.9)$$


Figure 7) The simulation time is discretized (top) and for each sub-region (blue) the Hamiltonian is time-averaged)

b) Matrix Exponentiation: The approximate sub-region evolution operators are the following:

$$\hat{U}_{\alpha,sub}^{(r)} = e^{-i\delta t \hat{H}_{sub}^{(r)}} \quad (3.10)$$

c) Sub-Region Evolution Operator Error: The eigenvalue spread is as follows (Equation 3.1). The notation $\max \tau$ indicates a maximum taken over time τ .

$$H = |\max\{\epsilon_{\alpha}(t)\} - \min\{\epsilon_{\alpha}(t)\}|_{\max \tau} \quad (3.11)$$

The sub-region error coefficient is the following:

$$E_{sub} = H\delta t \quad (3.12)$$

The error in the sub-region evolution operators is given by the Baker Campbell-Hausdorff formula [86]:

$$\hat{\mathcal{E}}_{sub}^{(r)} = 0 + O(E_{sub}^2) \quad (3.13)$$

C) Quantum-Simulation Computational Cost

The computational cost of TI-PFA is determined by counting the number of elementary operations [87].

1. Matrix Exponentiation

The approximate sub-region evolution operators are computed using a Λ -truncated Taylor series [88]:

$$\hat{U}_{a,sub}^{(r,\Omega)} = \sum_{n=0}^{\Lambda} \frac{(-i\hat{H}_{sub}^{(r)}\delta t)^n}{n!} \quad (3.14)$$

The number of matrix multiplications required for the computation is the following:

$$N_{Mult} = (\Lambda - 1) \quad (3.15)$$

2. Matrix Multiplication

Classical computers perform matrix multiplication by manipulating matrix elements:

$$(\mathbf{A} \times \mathbf{B})_{i,j} = \sum_{k=1}^d A_{i,k} B_{k,j} \quad (3.16)$$

The number of elementary operations required in the textbook matrix multiplication algorithm is as follows [87]:

$$N_{op.} = d^3 \quad (3.17)$$

The time-complexity is the length of time required for a computing algorithm to run to completion [87]:

$$\mathfrak{T}_c = t_{op} N_{op} \quad (3.18)$$

3. Computational Cost

a) Matrix Exponentiation Cost: The computational cost of approximating all of the sub-region evolution operators is the following:

$$\mathfrak{T}_c \left\{ \hat{U}_{a,sub}^{(r,\Lambda)} \right\} = (\Lambda - 1) L_{sim} t_{op} d^3 \quad (3.19)$$

b) Matrix Multiplication Cost: The computational cost of generating the ordered product is the following:

$$\mathfrak{T}_c \{ \text{Multiplication} \} = (L_{sim} - 1) t_{op} d^3 \quad (3.20)$$

c) Algorithm Cost: The computational cost of TI-PFA is the following:

$$\mathfrak{T}_c \{ \text{TI-PFA} \} = (\Lambda L_{sim} - 1) t_{op} d^3 \quad (3.21)$$

4. Quantum-Simulation Error

a) Algorithm Error: The error in TI-PFA is the following (Equation 3.13):

$$\epsilon_{TI-PFA} \square L_{sim} \hat{\mathcal{E}}_{sub}^{(r)} \quad (3.22)$$

$$\in_{TI-PFA} \square H \tau O(E_{sub}) \quad (3.23)$$

If the discretization condition holds, TI-PFA will achieve the target simulation error reliably:

$$L_{sim} \square \frac{H^2 \tau^2}{2 \epsilon_{target}} + \frac{H \tau}{2} \quad (3.24)$$

b) Minimum Algorithm Cost: The perturbative noise condition must hold for TI-PFA to converge (Equation 3.13):

$$E_{sub} < 1 \quad (3.25)$$

The perturbative noise condition sets the minimum step-number:

$$L_{sim} > H \tau \quad (3.26)$$

The minimum step-number is used to lower-bound the computational cost of TI-PFA (Equation 3.21):

$$T_c \{TI-PFA\} \geq \{ \Lambda \text{Max}(H \tau, 1) - 1 \} t_{op} d^3 \quad (3.27)$$

$$\geq \text{Max}(H \tau, 1) - 1 \} t_{op} d^3 \quad (3.28)$$

4. STROBOSCOPIC EXPONENTIATION ALGORITHM

The Stroboscopic Exponentiation Algorithm (SEA) leverages Hamiltonian periodicity for time-efficient quantum-simulation.

A) Stroboscopic Simulation

1. Periodic Hamiltonians

A periodic Hamiltonian has discrete time-translational symmetry with period T:

$$\hat{H}_{p,sim}(t+T) = \hat{H}_{p,sim}(t) \quad (4.1)$$

2. Stroboscopic Evolution Operator

The simulation time can be expressed as follows:

$$\tau = k \lambda T + \Delta t, k \in \mathbb{N}, \lambda \in \mathbb{N}_1 \quad (4.2)$$

Where $\mathbb{N}: \{0, 1, 2, \dots, \infty\}$ $\mathbb{N}_1: \{1, 2, \dots, \infty\}$

The periodic evolution operator obeys the following [89]:

$$\hat{U}_{p,sim}(\tau) = \{\hat{U}_{p,sim}(\Delta t)\}^k \{\hat{U}_{p,sim}(\lambda T)\}^k \quad (4.3)$$

3. Stroboscopic Simulation Algorithm

The stroboscopic simulation algorithm (SSA) can be represented schematically in two stages (Figure 8) [90]:

1. Aliasing: Obtain the base time-symmetry evolution operator and the remainder evolution operator.
2. Matrix Multiplication: Generate the periodic evolution operator using ordered products.

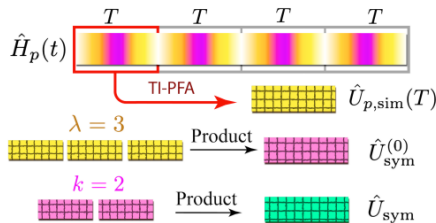


Figure 8) The periodic evolution operator is generated for one period (yellow). The base time-symmetry evolution operator (pink) and the time-symmetry evolution operator (green) are generated using matrix multiplication

a) Aliasing: The base time-symmetry evolution operator is the following:

$$\hat{U}_{sym}^{(0)} = \left[\tau \{ e^{-i \int_0^T dt' \hat{H}_{p,sim}(t')} \} \right]^\lambda \quad (4.4)$$

The remainder evolution operator is the following:

$$\hat{U}_{rem} = \tau \{ e^{-i \int_0^{\Delta t} dt' \hat{H}_{p,sim}(t')} \} \quad (4.5)$$

b) Matrix Multiplication: The time-symmetry evolution operator is the following:

$$\hat{U}_{sym} = \{\hat{U}_{sym}^{(0)}\}^k \quad (4.6)$$

The periodic evolution operator is the following:

$$\hat{U}_{p,sim}(\tau) = \{\hat{U}_{rem}\} \{\hat{U}_{sym}\} \quad (4.7)$$

4. Computational Cost

a) Aliasing Cost: The base time-symmetry evolution operator and the remainder evolution operator are both approximated with TI-PFA (Equation 3.28):

$$\tau_c \{U_{a,sym}^{(0)}\} \geq \{ \text{Max}(H, \tau, 1) + \lambda - 2 \} t_{op} d^3 \quad (4.8)$$

$$\tau_c \{U_{a,rem}^{(0)}\} \geq \{ \text{Max}(H \Delta t, 1) - 1 \} t_{op} d^3 \quad (4.9)$$

b) Matrix Multiplication Cost: The computational cost of generating the ordered product is the following:

$$\tau_c \{ \text{Multiplication} \} = k t_{op} d^3 \quad (4.10)$$

c) Minimum Algorithm Cost: The computational cost of SSA is lower-bounded by the following:

$$\tau_c \{SSA\} \geq \{ \text{Max}(H(T + \Delta t), 2) + (\lambda - 3) + k \} t_{op} d^3 \quad (4.11)$$

d) Parametrized Minimum Algorithm Cost: The computational cost of SSA can be parametrized as follows (Equation 4.2):

$$\tau_c \{SSA\} \geq \{ \text{Max}(H(T + \Delta t), 2) + (\lambda - 3) + \frac{\tau - \Delta t}{\lambda T} \} t_{op} d^3 \quad (4.12)$$

e) Quantum-Simulation Error: The error in SSA is the following (Equation III.23):

$$\in_{SSA} \square (k \lambda) \in_{TI-PFA} \quad (4.13)$$

$$\in_{SSA} \square (k \lambda) H T O(E_{sub}) \quad (4.14)$$

$$\in_{SSA} \square H T O(E_{sub}) \quad (4.15)$$

B) Stroboscopic Exponentiation Algorithm

1. Stroboscopic Evolution Operator

The simulation time can be expressed as follows:

$$\tau = k \lambda T + \Delta t, k \in \mathbb{N}, \lambda \in \mathbb{N}_1 \quad (4.16)$$

The integer k is expressed using binary notation [91]:

$$k = \sum_{n=0}^K k_n 2^n, k_n \in \{0,1\} \quad (4.17)$$

The periodic evolution operator obeys the following:

$$\hat{U}_{p,sim}(\tau) = \left\{ \hat{U}_{p,sim}(\Delta t) \right\}^{\left[\prod_{n=0}^K \left\{ \hat{U}_{p,sim}(2^n \lambda T) \right\}^{k_n} \right]} \quad (4.18)$$

2. Stroboscopic Exponentiation Algorithm

SEA can be represented schematically in three stages (Figure 9):

1. Aliasing: Obtain the base time-symmetry evolution operator and the remainder evolution operator.
2. Exponentiation: Perform recursive multiplication on the base time-symmetry evolution operator.
3. Matrix Multiplication: Generate the periodic evolution operator using ordered products.

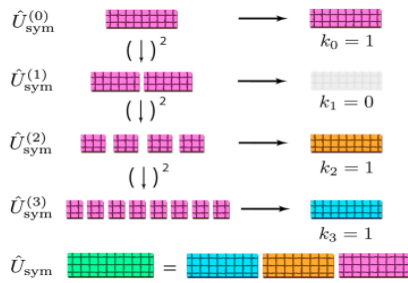


Figure 9) The exponentiated time-symmetry evolution operators are generated recursively (left). The binary decomposition (right) is used to generate the time-symmetry evolution operator (bottom).

a) Aliasing: The base time-symmetry evolution operator and remainder evolution operator are defined in Section 4 A 3 a)

b) Exponentiation: The exponentiated time-symmetry evolution operators are the following:

$$\hat{U}_{sym}^{(n)} = \left(\hat{U}_{sym}^{(0)} \right)^{2^n} \quad (4.19)$$

The exponentiated time-symmetry evolution operators are generated recursively:

$$\hat{U}_{sym}^{(n)} = \left(\hat{U}_{sym}^{(n-1)} \right)^2 \quad (4.20)$$

c) Matrix Multiplication: The time-symmetry evolution operator is as follows:

$$\hat{U}_{sym} = \prod_{n=0}^K \left\{ \hat{U}_{sym}^{(n)} \right\}^{k_n} \quad (4.21)$$

The periodic evolution operator is the following:

$$\hat{U}_{p,sim}(\tau) = \left\{ \hat{U}_{rem} \right\} \left\{ \hat{U}_{sym} \right\} \quad (4.22)$$

3. Computational Cost

a) Aliasing Cost: The base time-symmetry evolution operator and the remainder evolution operator are generated as in Section 4 A 4 a)

b) Exponentiation Cost: The computational cost of generating the exponentiated time-symmetry operators is the following:

$$\tau_c \left\{ \hat{U}_{sym}^{(n)} \right\} = K t_{op} d^3 \quad (4.23)$$

c) Matrix Multiplication Cost: The computational cost of generating the ordered product is the following:

$$\tau_c \{ Multiplication \} = \left(\sum_{n=0}^K k_n \right) t_{op} d^3 \quad (4.24)$$

d) Minimum Algorithm Cost: The computational cost of SEA is lower-bounded by the following:

$$\tau_c \{ SEA \} \geq \{ Max(H(T + \Delta t), 2) + (\lambda + K - 3) + \sum_{n=0}^K t_{op} d^3 \} \quad (4.25)$$

e) Binary Constraint: The binary decomposition constrains the number of exponentiated time-symmetry operators:

$$\lambda T 2^{(K+1)} > \tau - \Delta t \quad (4.26)$$

$$K > \log_2 \left(\frac{\tau - \Delta t}{2\lambda T} \right) \quad (4.27)$$

f) Parametrized Minimum Algorithm Cost: The computational cost of SEA can be parametrized as follows:

$$\tau_c \{ SEA \} \geq \{ Max(H(T + \Delta t), 2) + (\lambda - 3) + Max(\log_2 \left(\frac{\tau - \Delta t}{2\lambda T} \right), 0) t_{op} d^3 \} \quad (4.28)$$

4. Quantum-Simulation Error

The error in SEA is the following (Equation 4.15)

$$\epsilon_{SEA} = H \tau O(E_{sub}) \quad (4.29)$$

C) Algorithm Comparison

1. Asymptotic Cost Analysis

The asymptotic computational costs of the quantum simulation algorithms are the following:

$$\lim_{\tau \rightarrow \infty} T_c \{ TI-PFA \} \geq H \tau t_{op} d^3 \quad (4.30)$$

$$\lim_{\tau \rightarrow \infty} T_c \{ SSA \} \geq \frac{\tau}{\lambda T} t_{op} d^3 \quad (4.31)$$

$$\lim_{\tau \rightarrow \infty} T_c \{ SEA \} \geq \log_2 \left(\frac{\tau}{\lambda T} \right) t_{op} d^3 \quad (4.32)$$

a) Relative Algorithm Performance: SEA achieves an exponential speed-up over TI-PFA and SSA in simulating periodic Hamiltonians (Figure 10).

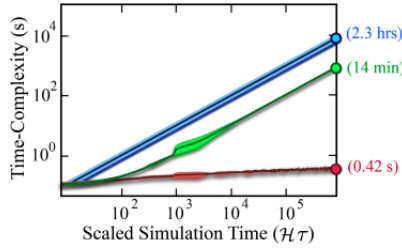


Figure 10) The computational cost required to apply TI-PFA (blue), SSA (green), and SEA (red) to a 10-qubit periodic Hamiltonian is empirically determined

5 TRAP SIM II

Trap Sim II is a proprietary MATLAB code that performs time-efficient quantum-simulation of ion trap quantum computers.

A) Hamiltonian Periodicity

1. Schrodinger Picture Hamiltonian

The laser period is the following:

$$T_{laser} = \frac{2\pi}{\omega} \quad (5.1)$$

The Schrodinger picture Hamiltonian is periodic:

$$\hat{H}_{ion trap}(t + T_{laser}) = \hat{H}_{ion trap}(t) \quad (5.2)$$

2. Interaction Picture Hamiltonian

The interaction picture Hamiltonian is not periodic in general (Equation 2.73).

B) Regularization Effects

1. Hamiltonian Regularization

A bosonic truncation is placed on the ladder operators [92-94]:

$$a_{\zeta}^{\dagger} |n\rangle = 0, \forall n \geq \zeta \quad (5.3)$$

The regularized effective ion trap Hamiltonian is the following (Equation 2.68):

$$\hat{H}_{eff, ion trap}^{(\zeta)}(t) = \sum_{k=1}^{3N} \omega_k \{ \hat{a}_k^{\dagger} a_k^{\zeta} \} + \hat{H}_{qubit}(t) \quad (5.4)$$

2. Computer Memory

The dimension of the Hilbert space is the following:

$$\dim\{\hat{H}_{ion trap}\} = 2^N (\zeta + 1)^{3N} \quad (5.5)$$

The memory required to perform quantum-simulation on a 64-bit processor is the following (Figure 11):

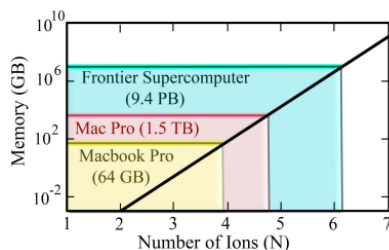


Figure 11) The threshold simulation memory (black) is compared with the random access memory of several classical computing platforms (colored) [96-

98].

$$\text{Memory}\{\hat{H}_{ion trap}\} = 16 \text{ bytes} \times 4^N (\zeta + 1)^{6N} \quad (5.6)$$

3. Bosonic Saturation

The vibrational occupation operators are as follows [95]:

$$\hat{N}_k = \hat{a}_k^{\dagger} \hat{a}_k \quad (5.7)$$

The vibrational occupation uncertainties are as follows:

$$\sigma_{N_k} = \sqrt{\langle \hat{N}_k^2 \rangle - \langle \hat{N}_k \rangle^2} \quad (5.8)$$

If the bosonic truncation is saturated, an accumulation of regularization effects ensure that the simulation can no longer be compared to nature:

$$\text{Bosonic Saturation: } \langle \hat{N}_k \rangle \pm \sigma_{N_k} \square \zeta \quad (5.9)$$

C) Anisotropic Randomized Truncation

Anisotropic Randomized Truncation (ART) is used to estimate the size of regularization effects. It can be represented schematically in three stages:

1. Truncation: Regularize the Hamiltonian randomly.
2. Quantum-Simulation: Generate an evolution operator for the regularized Hamiltonians.
3. Error-Estimation: Estimate the regularization effects using quantum channel technology.

1. Truncation

The vibrational modes are regularized anisotropically (Figure 12):

$$\hat{H}_{eff, ion trap}^{(\vec{\zeta})}(t) = \sum_{k=1}^{3N} \omega_k \{ \hat{a}_k^{\dagger} a_k^{\zeta_k} \} + \hat{H}_{qubit}(t) \quad (5.10)$$

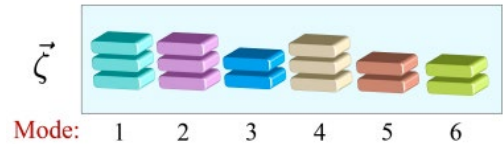


Figure12) The maximum number of vibrational excitations (colored) is set independently for each mode

Regularized Hamiltonians are selected pseudorandomly to generate the ART Hamiltonian set:

$$A_H = \{ \hat{H}_{eff, ion trap}^{(\zeta_1)}(t), \dots, \hat{H}_{eff, ion trap}^{(\zeta_{Na})}(t) \} \quad (5.11)$$

2. Quantum-Simulation

a) Regularized Evolution Operators: The regularized evolution operators are the following:

$$\hat{U}_{reg}(\vec{\zeta}) = T \left\{ e^{-i \int_0^T dt' \hat{H}_{eff, ion trap}^{(\vec{\zeta})}(t')} \right\} \quad (5.12)$$

b) Haar Measure: The regularized Haar measure is a subset of the Haar measure composed of the regularized evolution operators (Figure 13) [96-100]:



Figure 13) ART generates unitary operators (red) from the regularized Haar measure (gray), which contains the ideal evolution operator (blue).

$$U_{reg} = \{\hat{U}_{reg}(\vec{\zeta}), \forall \vec{\zeta}\}, \quad (5.13)$$

$$U_{reg} \subseteq U_{Haar} \quad (5.14)$$

The ART unitary set is the following:

$$A_u = \{\hat{U}_{reg}(\vec{\zeta}_1), \dots, \hat{U}_{reg}(\vec{\zeta}_{N_a})\} \quad (5.15)$$

$$A_u \subseteq U_{reg} \quad (5.16)$$

3. Error-Estimation

Simulated Expectation-Value Approximate Reconstruction (SEAR) is used to approximate the regularization effects [101].

a) Quantum Channel Technology: A superoperator on a Hilbert space H has the following form [102]:

$$\mathcal{E} = \sum_{\mu=1}^R \hat{K}_{\mu} \otimes \hat{K}_{\mu}^{\dagger} \quad (5.17)$$

$$\hat{K}_{\mu} \in H \otimes H^* \quad (5.18)$$

A quantum channel is a type of super operator. Its Kraus operators satisfy the following condition [103,104]:

$$\sum_{\mu=1}^R \hat{K}_{\mu} \hat{K}_{\mu}^{\dagger} = \hat{1} \quad (5.19)$$

The action of a quantum channel on a state $|\psi\rangle$ generates a density matrix [105, 106]:

$$\mathcal{E}(|\psi\rangle) = \sum_{\mu=1}^R \hat{K}_{\mu} |\psi\rangle \langle\psi| \hat{K}_{\mu}^{\dagger} \quad (5.20)$$

b) Quantum Channel Averaging: Applying a similarity transformation to a quantum channel yields the following [107]:

$$\mathcal{E}_u = U^{\dagger} \mathcal{E} U \quad (5.21)$$

$$= \sum_{\mu=1}^R \hat{U}^{\dagger} \hat{K}_{\mu} \hat{U} \otimes \hat{U}^{\dagger} \hat{K}_{\mu}^{\dagger} \hat{U} \quad (5.22)$$

Averaging a quantum channel over the Haar measure yields a depolarizing channel (Figure 14) [107, 108]:

$$D_{\epsilon} = \int dU_{Haar} U^{\dagger} \mathcal{E} U \quad (5.23)$$

$$D_{\epsilon}(\rho) = (1-\epsilon)\rho + \epsilon \frac{1}{\dim(H)} \quad (5.24)$$

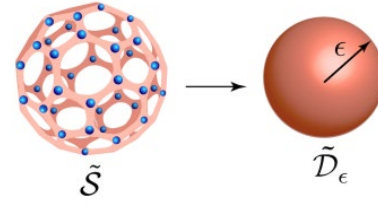


Figure 14) The SEAR error channel (left) is defined using its kraus operators (blue). Averaging the SEAR error channel generates a depolarizing channel (right).

The depolarizing channel has characteristic noise strength [109–116]:

$$\epsilon = 1 - \frac{\text{Tr}(\mathcal{E}) - 1}{[\dim(H)]^2 - 1} \quad (5.25)$$

$$0 \leq \epsilon \leq 1 \quad (5.26)$$

c) Approximate Quantum Simulation: The ideal evolution operator has an arbitrarily large bosonic truncation (Figure 13):

$$\hat{U}_{ideal} = \hat{U}_{reg}(\infty) \quad (5.27)$$

The ideal output state is the following:

$$\rho_{ideal} = \hat{U}_{ideal} (|\psi\rangle \langle\psi|) \hat{U}_{ideal}^{\dagger} \quad (5.28)$$

The regularized output states are the following:

$$\rho_{reg}^{(\vec{\zeta})} = \hat{U}_{reg}(\vec{\zeta}) (|\psi\rangle \langle\psi|) \hat{U}_{reg}(\vec{\zeta})^{\dagger} \quad (5.29)$$

Averaging the regularized output states generated by the ART unitary set yields the ART output state:

$$\rho_{ART} = \frac{1}{N_a} \sum_{\mu=1}^{N_a} \rho_{reg}^{(\vec{\zeta}_{\mu})} \quad (5.30)$$

d) SEAR Error Channel: The SEAR error channel maps the ideal output state to the ART output state:

$$\mathcal{S}(\rho_{ideal}) = \rho_{ART} \quad (5.31)$$

The SEAR error channel is written explicitly:

$$\mathcal{S} = \frac{1}{N_a} \sum_{\mu=1}^{N_a} \hat{U}_{SEAR}(\vec{\zeta}_{\mu}) \otimes \hat{U}_{SEAR}(\vec{\zeta}_{\mu})^{\dagger} \rightarrow \quad (5.32)$$

$$\hat{U}_{SEAR}(\vec{\zeta}_{\mu}) \rightarrow \hat{U}_{reg}(\vec{\zeta}_{\mu}) \hat{U}_{ideal}^{\dagger} \quad (5.33)$$

The SEAR noise strength is the following:

$$\epsilon_{SEAR} = 1 - \frac{\text{Tr}(\mathcal{S}) - 1}{[\dim(H)]^2 - 1} \quad (5.34)$$

e) Regularization Effects: The SEAR error channel forces observables to stray from their ideal values, causing truncation fluctuations:

$$\Delta O_{trunc} = |\langle\psi| \hat{U}_{ideal}^{\dagger} \hat{O} \hat{U}_{ideal} |\psi\rangle - \text{Tr}\{\mathcal{S}(\rho_{ideal}) \hat{O}\}| \quad (5.35)$$

The average truncation fluctuation can be bounded using the SEAR noise strength [101]:

$$\overline{\Delta O}_{trunc} \leq \epsilon_{SEAR} |O_{eigenvalue}^{\max} - O_{eigenvalue}^{\min}| \quad (5.36)$$

f) Noise Spectroscopy: The complementary SEAR error channels are generated by substituting the ideal evolution operator with the regularized evolution operators (Equation 5.33). The SEAR error channel cannot be studied directly due to the inaccessibility of the ideal evolution operator:

$$\hat{S}_\eta = \frac{1}{N_a} \sum_{\mu=1}^{N_a} \hat{U}_{SEAR}^{(n)}(\vec{\zeta}_u) \otimes \hat{U}_{SEAR}^{(n)\dagger}(\vec{\zeta}_u) \frac{\partial^2 \Omega}{\partial u^2} \quad (5.37)$$

$$\hat{U}_{SEAR}^{(\eta)}(\vec{\zeta}_u) \rightarrow \hat{U}_{reg}(\vec{\zeta}_u) \hat{U}_{reg}^\dagger(\vec{\zeta}_\eta) \quad (5.38)$$

The complementary SEAR noise strength can be estimated using measurement protocols [101, 108].

D) Numerical Results

Trap Sim II is used to simulate an ion trap quantum computer.

a) Simulation Goals: The simulation is performed to examine the following:

1. Bosonic Saturation
2. Regularization Effects
3. Entanglement Growth
4. Weak-Laser Approximation (WLA)

b) Simulation Parameters: The simulation parameters are the following [42, 43]:

$$\text{Number of Ions: } N = 1 \quad (5.39)$$

$$\text{Ion Charge: } Q = +e \quad (5.40)$$

$$\text{Ion Mass: } M \sim 200 \text{ GeV} \quad (5.41)$$

$$\text{Physical Trap Frequency: } \omega_a \sim 1 \text{ MHz} \quad (5.42)$$

$$\text{Laser Wavelength: } \lambda \sim 400 \text{ nm} \quad (5.43)$$

$$\text{Laser Power: } P_{\text{laser}} \sim 1 \text{ W} \quad (5.44)$$

$$\text{Bosonic Truncation: } \zeta \sim 6 \quad (5.45)$$

$$\text{Trap Potential: XY-Symmetric \& Harmonic} \quad (5.46)$$

c) Numerical Results

a) Bosonic Saturation: The vibrational occupation is computed throughout the simulation (Figure 15, Figure 16).

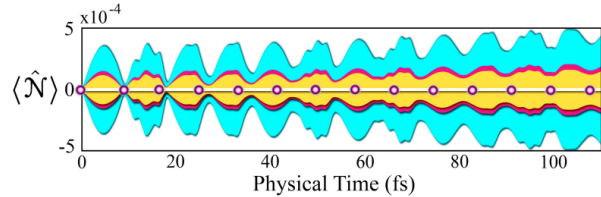


Figure 15) On the laser timescale, the vibrational occupation of the X-mode (magenta), the Y-mode (yellow), and the Z-mode (cyan), fluctuates non-trivially around zero. (The uncertainty is amplified by a factor of 104. The observable is sampled 7.5 times faster than displayed)

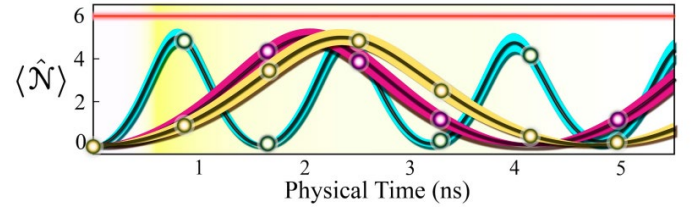


Figure 16) The vibrational occupation of the modes grows until the bosonic truncation (red) is approached. The onset of bosonic saturation (yellow backdrop) results in unphysical oscillations of the vibrational occupation. (The uncertainty is suppressed by a factor of 3. The observable is sampled 7.5 times faster than displayed).

Computational Details:

- The ion trap is initialized in the motional groundstate [117–134].

b) Regularization Effects: The SEAR noise strength is approximated using ART (Figure 17, Figure 18).

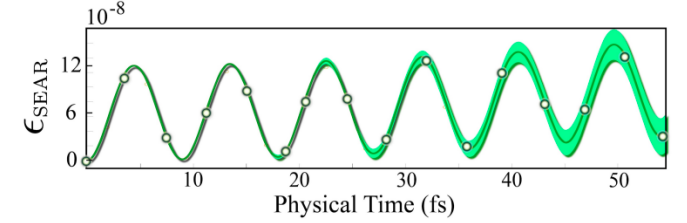


Figure 17) On the laser timescale, the SEAR noise strength (green) is perturbative small, indicating the initial accuracy of the quantum-simulation protocol. (The uncertainty is amplified by a factor of 8×10^4 . The observable is sampled 3 times faster than displayed).

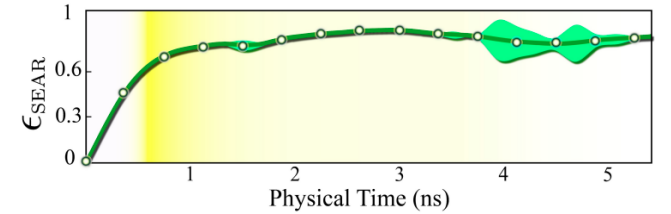


Figure18) The SEAR noise strength (green) approaches unity after the onset of bosonic saturation (yellow backdrop), indicating the ultimate failure of the quantum-simulation protocol. (The uncertainty is amplified by a factor of 5×10^2 . The observable is sampled 3 times faster than displayed).

Computational Details:

- Eight anisotropic bosonic truncations are chosen.
- The SEAR noise strength is estimated repeatedly.
- A bootstrap algorithm is used to generate uncertainty in the average SEAR noise strength estimate [135, 136].

c) Entanglement Growth: The von Neumann entanglement entropy of the qubit is computed throughout the simulation (Figure 19, Figure 20). Entanglement entropy is a wildly important quantity, with applications to many areas of physics [137–193].

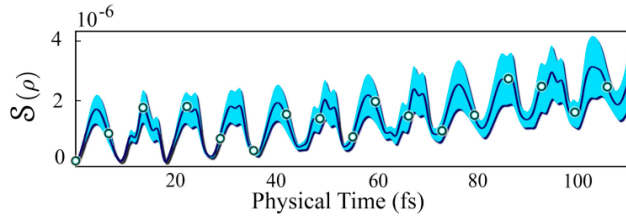


Figure 19) On the laser timescale, the entanglement entropy (blue) fluctuates non-trivially as the qubit interacts with the vibrational modes. (The uncertainty is amplified by a factor of 2. The observable is sampled 6 times faster than displayed)

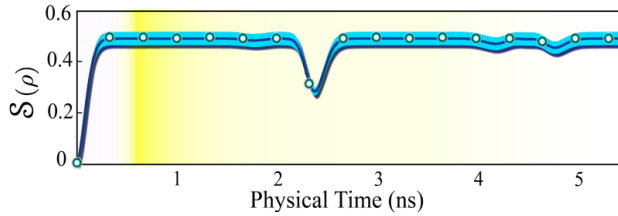


Figure 20) The entanglement entropy (blue) ceases to grow after the onset of bosonic saturation (yellow backdrop), and the decoherence of the qubit is halted) (The observable is sampled 6 times faster than displayed).

$$s(\rho) = -\text{Tr}(\rho \log(\rho)) \quad (5.47)$$

Computational Details:

- The qubit is initialized in 10^2 pseudo-randomly generated pure states [104].
- A bootstrap algorithm is used to generate an uncertainty in the average entanglement entropy.

d) Effective Hamiltonian Validity: The WLA error is computed (Figure 21, Figure 22).

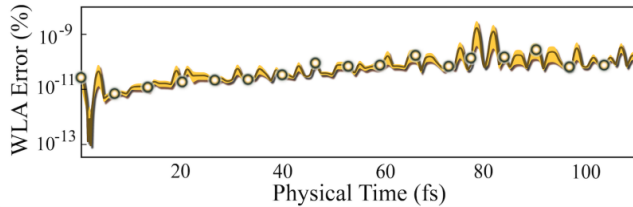


Figure 21) Over the laser timescale, the WLA error (golden) increases by several orders of magnitude) (The observable is sampled 6 times faster than displayed).

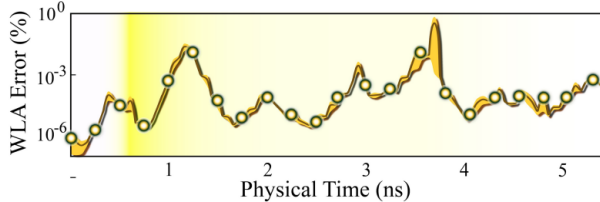


Figure 22) The WLA error (golden) fluctuates non-trivially after the onset of bosonic saturation (yellow backdrop). (The observable is sampled 6 times faster than displayed)

Computational Details:

- The qubit is initialized in 10^2 pseudo-randomly generated pure states.
- The Pauli operator $\hat{\sigma}_z$ is measured)
- A bootstrap algorithm is used to generate an uncertainty in the average WLA error.

4. Empirical Observations

a) Bosonic Saturation: After the onset of bosonic saturation, the vibrational occupation exhibits unphysical behavior (Figure 16). Commentary:

- Bosonic saturation places a temporal limit on the amount of ion trap dynamics that can be probed numerically.
- This suggests that ion trap quantum-simulation be used as a performance heuristic for quantum-simulation protocols [194].
- The (N, ζ, ϵ) ion-trap performance heuristic is the following:

A quantum-simulation protocol passes the (N, ζ, ϵ) ion-trap performance heuristic by performing quantum-simulation of the N -ion, ζ -cutoff ion trap Hamiltonian until bosonic saturation is observed, with total error bounded by ϵ .

b) Regularization Effects: The noise strength increases with simulation time, and experiences a sharp growth during the onset of bosonic saturation (Figure 18). Commentary:

- Each ART Hamiltonian generates a different set of regularization effects due to the anisotropic bosonic truncation.
- The SEAR noise strength provides a measure of the disparity between the ART unitary operators (Equation 5.33).
- The ART unitary operators diverge during bosonic saturation, and the average error grows to $\geq 60\%$.

c) Entanglement Growth: The entanglement entropy of the qubit increases with simulation time until the onset of bosonic saturation. The entanglement entropy then fluctuates non-trivially (Figure 20).

Commentary:

- The entanglement entropy is expected to increase as the purity of the qubit is lost to the environment [195–201].
- Bosonic saturation restricts the decoherence times that can be probed numerically [202]: Decoherence cannot be observed numerically unless the qubits are sufficiently noisy.

d) Effective Hamiltonian Validity: WLA accumulates $\sim 1\%$ error after the onset of bosonic saturation (Figure 22).

Commentary:

- The stability of approximations such as the rotating-wave approximation, the Lamb-Dicke limit, and the Magnus Expansion may be uncertain in the parameter regimes required for the most ambitious ion trap quantum computing proposals [237–246]. Much of the pressing uncertainty is rooted in the intractability of the Magnus Expansion [247].
- To conserve the limited and transient resources available to the scientific community at large, it is necessary to verify that perturbative protocols will succeed when implemented on real ion trap quantum computers, which are inherently nonperturbative) For a successful instance of this paradigm, see [248, 249].
- Trap Sim II is a rigorous algorithm test-bed for up to six ions (Figure 11). The sole approximation made by Trap Sim II is that of

finite bosonic truncation.

6. APPENDIX

A) TI-PFA vs. Sampling PFA

The sampling product-formula algorithm (S-PFA) [50, 90] can be expressed schematically in two stages:

1. Sampling: Sample the Hamiltonian at set times and approximates the sub-region evolution operators.
2. Matrix Multiplication: Take the ordered product of the approximate sub-region evolution operators.

a) Sampling

The sub-region Hamiltonians are as follows (Equation 3.9):

$$\hat{H}_{sub}^{(r)} = \hat{H}_{sim}((r-1)\delta t) \quad (6.1)$$

The approximate sub-region evolution operators are the following:

$$\hat{U}_{a,sub}^{(r)} = e^{-i\delta t \hat{H}_{sub}^{(r)}} \quad (6.2)$$

b) Sub-Region Evolution Operator Error

The maximum eigenvalue derivative of the Hamiltonian is the following:

$$D_{\max} = \left\{ \left| \frac{\partial}{\partial t} \varepsilon_{\alpha}(t) \right|_{\max} \right\}_{\max_{\tau}} \quad (6.3)$$

The error in the sub-region evolution operator is the following:

$$\varepsilon_{sub}^{(r)} \leq D_{\max} \delta t + O(E_{sub}^2) \quad (6.4)$$

c) Relative Algorithm Performance

S-PFA struggles to resolve the true dynamics of the Hamiltonian due to sampling errors, which are not present in TI-PFA [83-85].

B) Regularization Effects

If the length-scale of the laser is sufficiently long, the severity of the regularization effects can be determined rigorously via an efficient classical computation [250].

ACKNOWLEDGEMENT

Unjustly condemned, he was led away.

No one cared that he died without descendants, that his life was cut short in midstream. But he was struck down for the rebellion of my people)

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