Digital Quantum Simulation with Trapped Ions

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Outline

- Classical Simulation
- Quantum Simulation: Analog vs Digital
- Digital Quantum Simulation
- Implementation using trapped-ion quantum information
- Molmer-Sorensen Gate
- Experimental Results
- Experimental Limitations

Simulating Quantum Systems

- Goal of quantum Simulation: $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(t=0)\rangle$

- Some important applications for quantum simulation:

1. quantum magnetism in condensed matter

2. understand and design new materials

3. high-temperature superconductivity

Classical Simulation

- to compute exact dynamics $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi(t=0)\rangle$
  complexity is exponential in system size

- because dimensions of vector space is exponential in system size

- Example: 40 spin-1/2 particles
  state dimensions = 2^{40}
  evolution requires exponentiation of 2^{40} by 2^{40} matrix

- Just to store state of the system already requires exponentially many bits.

Classical Simulation

- What about using approximate numerical schemes? e.g. Path Integral Monte-Carlo simulation

- The issue is the numerical sign problem:
  integral of highly oscillatory functions requires extreme precision to obtain useful information.

- this situation is often encountered for strongly interacting fermions

- Classically, we need to confront the exponential complexity

Quantum Simulation

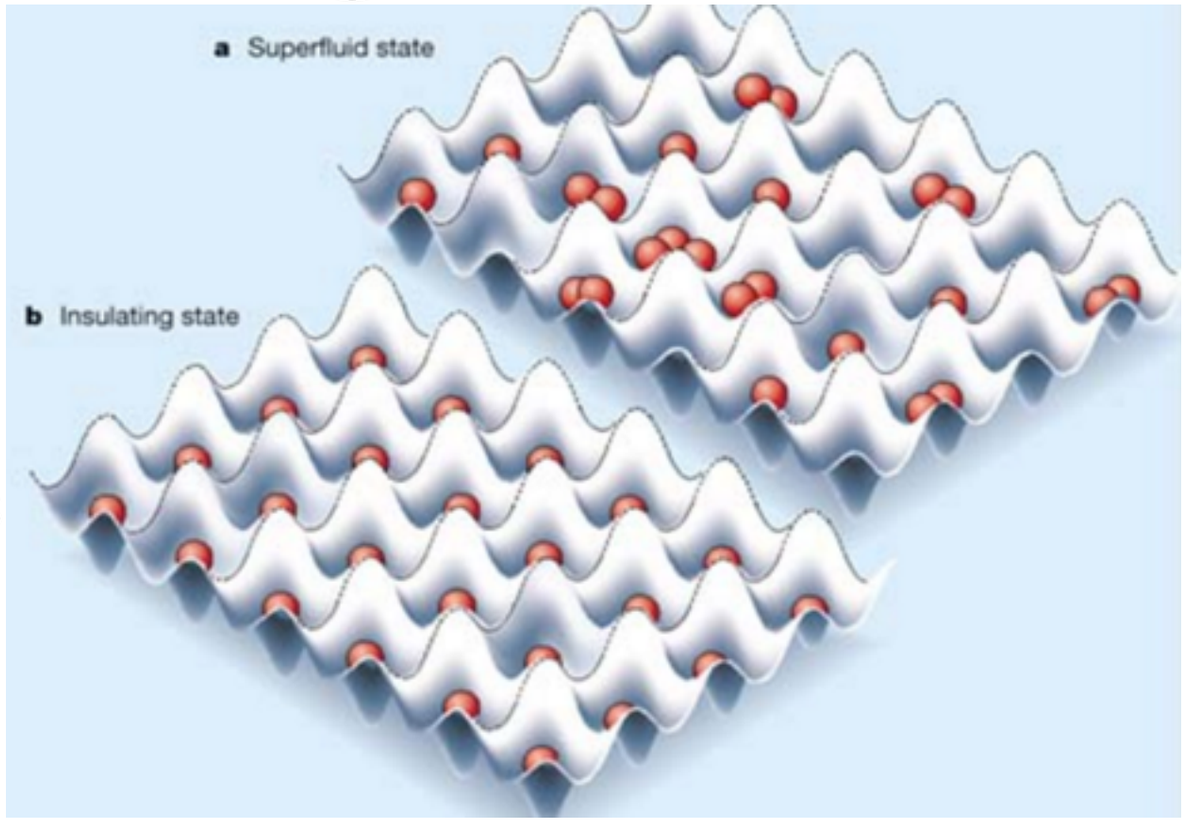
- Alternative approach by Feynman 1982
  “Use one quantum system to simulate another”

- Basic procedure:
  1. map variables to the simulator
  2. prepare the starting state
  3. evolve
  4. measure some quantity of interest

- immediately we see some advantage: only need O(N) qubits to simulate a N particle system

Analog vs Digital

- Analog Quantum Simulator:
  map directly the system to be simulated onto the simulator, i.e quantum emulator.
  e.g. simulating solid state physics using cold atoms in optical lattice



- Digital Quantum Simulator:
  use qubits to encode system and use gates to mimic the evolution
  e.g use two qubits per lattice site to number and spin of fermions present.

Digital Simulator

Recap:
1. encode system into qubits
2. apply sequence of gates to mimic evolution

Can we efficiently simulate any evolution? Not really.

- The simulator can be modelled as turning on and off a set of hamiltonians, e.g $\{\hat{H}_a, \hat{H}_b\}$

$$\hat{U} = \cdots e^{i\hat{H}_b t_4} e^{i\hat{H}_a t_3} e^{i\hat{H}_b t_2} e^{i\hat{H}_a t_1}$$

- In principle, if we have a universal set of gate operations, we can create any unitary to arbitrary accuracy.
- But in general, to create an arbitrary 2^N x 2^N unitary we need order 2^{2N} operations.
- So even though we can efficiently store the state of system, the simulation is still an exponentially hard problem

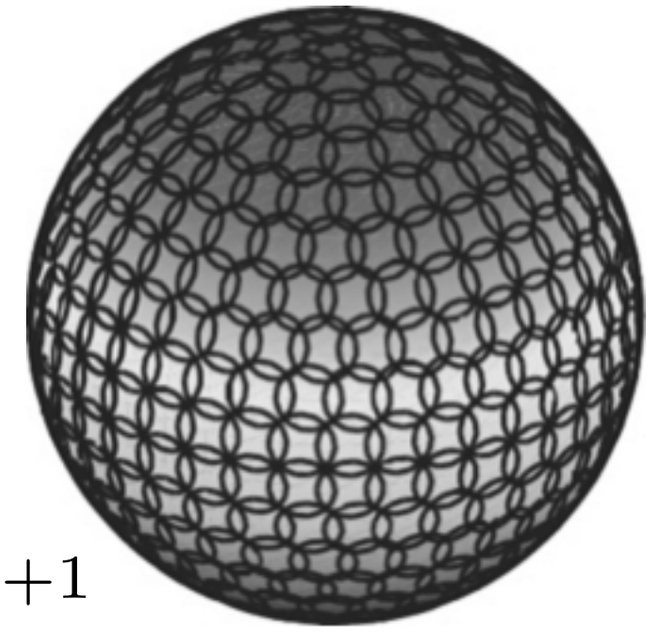
Approximating an arbitrary unitary is generically hard

Given a universal set of *g* gates which acts on at most *f* qubits, how many gates does it take to generate an arbitrary *n* qubit unitary?

- if we can generate an arbitrary unitary then we can starting from a fixed state generate an arbitrary n-bit state.
- so the question becomes: how many gates does it take to generate an arbitrary state.
- starting from $|0\rangle^{\otimes n}$, for each gate we can create at most $g\binom{n}{f} = O(n^f)$ states
- therefore, with *m* gates we have at most $O(n^{fm})$ states

Continued…

Acting on n bits with m gates from a set of g gates which act on at most f bits we can create at most $O(n^{fm})$ states



- suppose we wish to approximate to accuracy ϵ
- cover the space of states with ‘patches' of radius ϵ
- for n-qubits, dim = 2^n
- considering real and imaginary, dim = 2^{n+1}
- including the normalisation, states lie on surface of unit sphere in 2^{n+1} dimensions
- number of patches of radius ϵ is $\Omega(\frac{1}{\epsilon^{2^{n+1}-1}})$
- to reach all the patches, $O(n^{fm}) \geq \Omega(\frac{1}{\epsilon^{2^{n+1}-1}})$

$$\implies m = \Omega(\frac{2^n log(1/\epsilon)}{log(n)})$$

There are states or unitaries which take exponentially many gates to approximate within distance ϵ

What can we simulate?

- Local interactions.
  i.e. $\sum_i \hat{H}_i$ where each term involves at most k particles.

- example: Ising Model for ferromagnetism

$$J \sum_{\langle ij \rangle} \sigma_x^i \sigma_x^j + B \sum_i \sigma_z^i$$

XY Model

$$J_{xx} \sum_{\langle ij \rangle} \sigma_x^i \sigma_x^j + J_{yy} \sum_{\langle ij \rangle} \sigma_y^i \sigma_y^j + B \sum_i \sigma_z^i$$

- Not really a limitation since physical systems mostly only consist of local interactions.

How to efficiently simulate local interactions?

- Idea based on Trotter formula.

$$
\begin{aligned}
e^{-i\Delta t(\hat{H}_a+\hat{H}_b)} &= 1 - i\Delta t(\hat{H}_a + \hat{H}_b) + O(\Delta t^2) \\
&= e^{-i\Delta t\hat{H}_a} e^{-i\Delta t\hat{H}_b} + O(\Delta t^2)
\end{aligned}
$$

$$
\begin{aligned}
e^{-it(\hat{H}_a+\hat{H}_b)} &= \left[e^{-i\hat{H}_a t/n} e^{-i\hat{H}_b t/n} + O((t/n)^2)\right]^n \\
&= \left[e^{-i\hat{H}_a t/n} e^{-i\hat{H}_b t/n}\right]^n + O(t^2/n)
\end{aligned}
$$

- In general,

$$
e^{-it\sum_{i=1}^{l}\hat{H}_i} = \left[e^{-\hat{H}_1 t/n}\ldots e^{-\hat{H}_l t/n}\right]^n + O(t^2/n)
$$

Higher order Trotter approx.

- Trotter - Suzuki formula

$$e^{-i(\hat{H}_a+\hat{H}_b)t} = \left[e^{-i\hat{H}_b t/2n} e^{-i\hat{H}_a t/n} e^{-i\hat{H}_b t/2n}\right]^n + O(t^3/n^2)$$

- better error scaling

- can go to even higher orders for improved scaling

$$e^{-iH_a\alpha_1 t/n} e^{-iH_b\beta_1 t/n} e^{-iH_a\alpha_2 t/n} e^{-iH_b\beta_2 t/n} \ldots$$

Number of exponentials	α_1	β_1	α_2	β_2	α_3	β_3	α_4	O
2	1	1						$\frac{1}{N}$
3	$\frac{1}{2}$	1	$\frac{1}{2}$					$\frac{1}{N^2}$
4	$1-\gamma$	$\frac{1}{2\gamma}$	γ	$1-\frac{1}{2\gamma}$				$\frac{1}{N^2}$
5	$\frac{3\pm i\sqrt{3}}{12}$	$\frac{3+i\sqrt{3}}{6}$	$\frac{1}{2}$	$\frac{3\mp i\sqrt{3}}{6}$	$\frac{3\mp i\sqrt{3}}{12}$			$\frac{1}{N^3}$
6	$1-\gamma$	$\frac{1}{2\gamma}\frac{\frac{4}{3}-\gamma\pm\Gamma}{\gamma\pm\Gamma}$	$\frac{\gamma\pm\Gamma}{2}$	$\frac{1}{2}\frac{3-4\gamma}{2-3\gamma}$	$\frac{\gamma\mp\Gamma}{2}$	$1-\frac{1}{2\gamma}\frac{3\gamma-\frac{4}{3}\mp\Gamma}{\gamma\mp\Gamma}$		$\frac{1}{N^3}$
7	$\frac{\beta_1}{2}$	$\frac{1}{2-2^{1/3}}$	$\frac{1-2^{1/3}}{2}\beta_1$	$-2^{1/3}\beta_1$	$\frac{1-2^{1/3}}{2}\beta_1$	$\frac{1}{2-2^{1/3}}$	$\frac{\beta_1}{2}$	$\frac{1}{N^4}$

What is the efficiency now?

Trotter Formula:

$$e^{-it\sum_{i=1}^{l}\hat{H}_i} = \left[e^{-\hat{H}_1 t/n}\dots e^{-\hat{H}_l t/n}\right]^n + O(t^2/n)$$

- each term $e^{-\hat{H}_i t/n}$ requires at most $O(m^2)$ operations

- therefore, to an accuracy ϵ we need $nl(N)m^2$ operations.

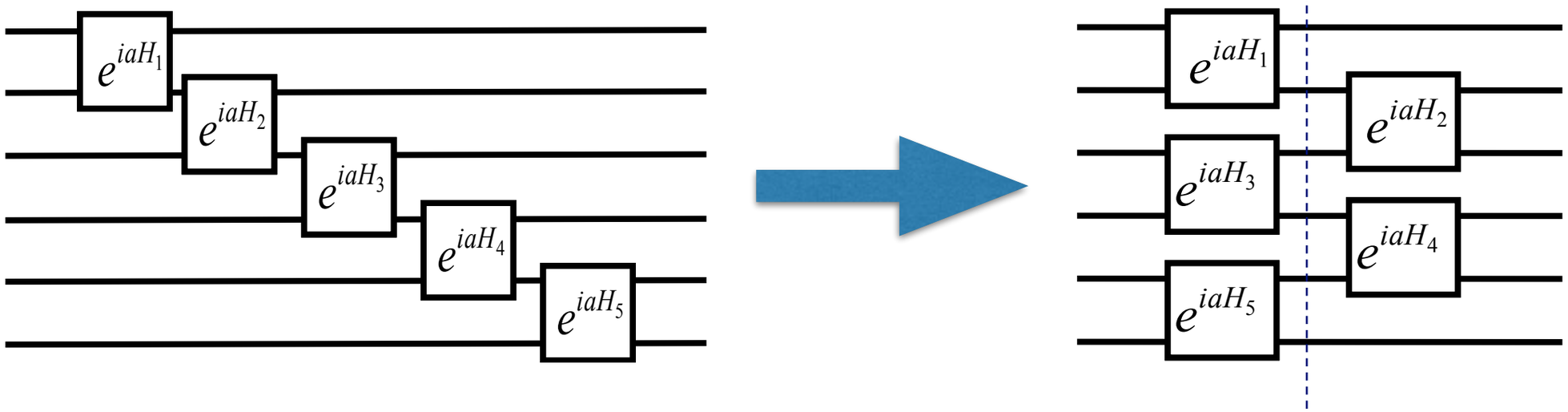
- so if l is polynomial in N, which is typical for local interactions. e.g. nearest neighbour interaction, $l \propto N$

- we have overcome the exponential scaling.

Parallelisation

$$e^{-it\sum_{i=1}^{l}\hat{H}_i} = \left[e^{-\hat{H}_1 t/n}\dots e^{-\hat{H}_l t/n}\right]^n + O(t^2/n)$$

- if we perform each term in sequence time complexity it would scale as $l(N)n$
- however, terms in the sum $\sum \hat{H}_i$ that commute can be applied simultaneously
- group the terms which commute among themselves
- since interaction is local, the number of groups is independent of system size
- so the time taken for the simulation is also independent of system size



Outlook

- the world is still a long way from a fully fledged quantum computer

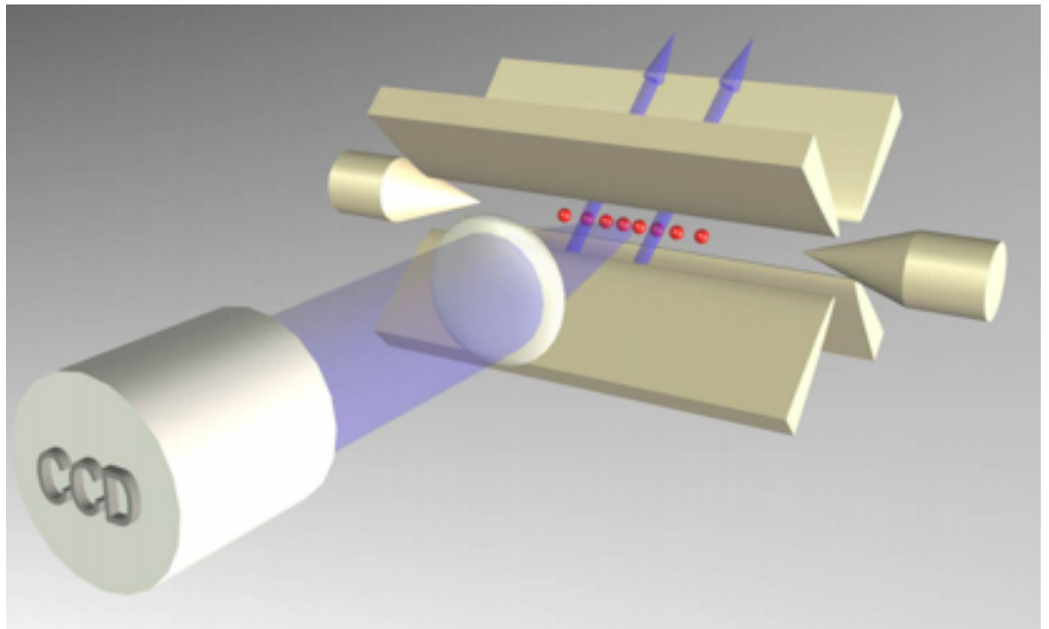
- for example, to factorise a 100-digit number using Shor's algorithm would require millions of logical operations performed without errors.

- on the other hand, with just few tens or hundreds of operations, it is possible to simulate a quantum system that would already take a classical computer Avogadro's number of operations

- quantum simulators are an exciting mid-term goal

Trapped Ion Quantum Simulator

- A string of $^{40}Ca^{+}$ ions loaded into a linear Paul trap

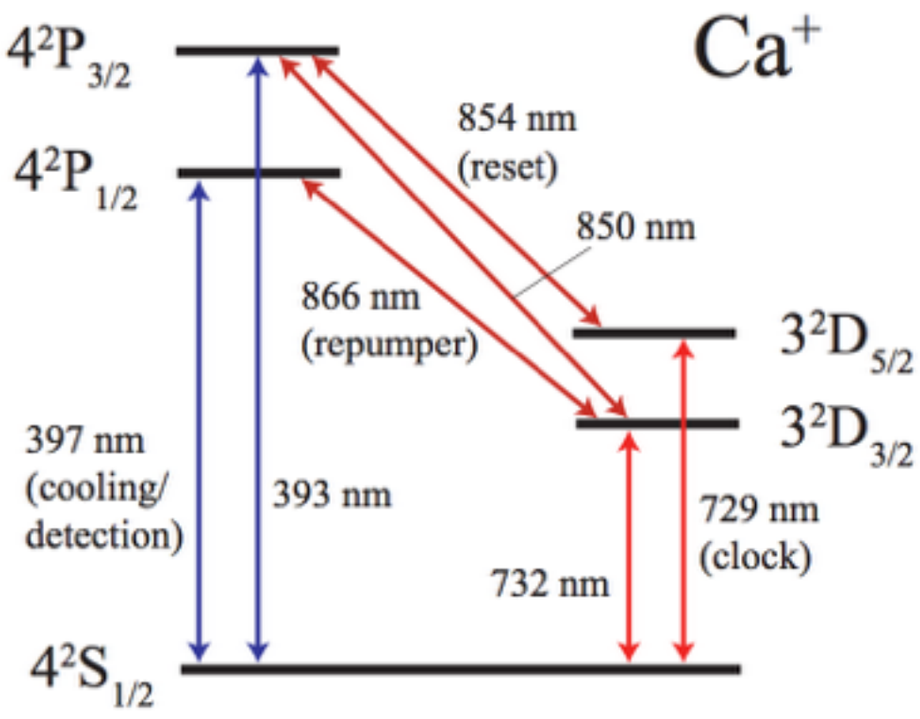


- Qubits encoded as such:
  excited state $|\uparrow\rangle = |\, D_{5/2}, m_j = -1/2\rangle$
  ground state $|\downarrow\rangle = |\, S_{1/2}, m_j = -1/2\rangle$

- Doppler cooled at the start on the 397nm transition

- Optical pumping and resolved sideband cooling prepares the qubit in the $|\downarrow\rangle$ state and vibrational ground state

- Detection: fluorescence detection using the 397nm transition

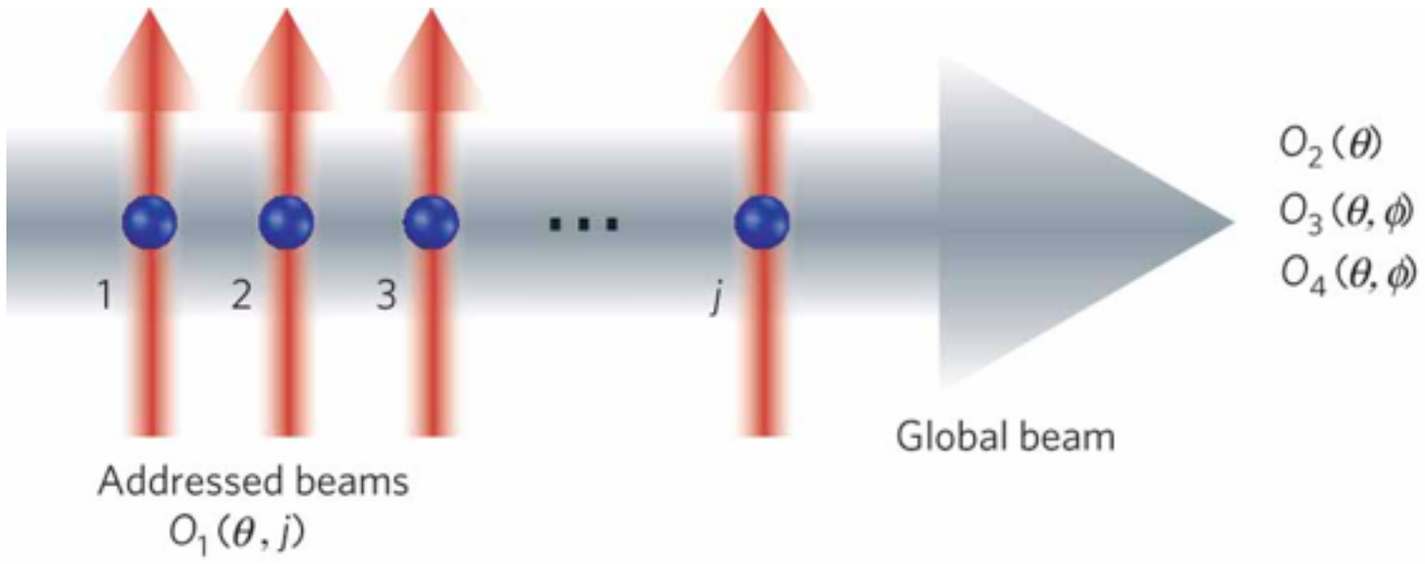


Universal Operation Set

Operation	Implementation
$O_1(\theta, i) = e^{-i\,\theta\,\sigma_z^i}$	detuned light field induces an AC-Stark effect given by the Hamiltonian $H = \frac{\hbar\Omega^2}{4\Delta}\sigma_z^i$ (Addressed Beam)
$O_2(\theta) = e^{-i\theta\,\sum_i \sigma_z^i}$	detuned light field induces an AC-Stark effect given by the Hamiltonian $H = \frac{\hbar\Omega^2}{4\Delta}\sum_i \sigma_z^i$ (Global Beam)
$O_3(\theta, \phi) = e^{-i\theta\,\sum_i \sigma_\phi^i}$	resonant laser pulse drives transition given by the Hamiltonian $H = \hbar\Omega\sigma_\phi^i$ (Global Beam)
$O_4(\theta, \phi) = e^{-i\theta\,\sum_{i<j} \sigma_\phi^i \sigma_\phi^j}$	global beam used with a bichromatic laser pulse to apply Molmer-Sorensen type interaction (Global Beam)

$$\sigma_\phi = cos\phi\sigma_x + sin\phi\sigma_y$$

$$\theta = Et/\hbar$$

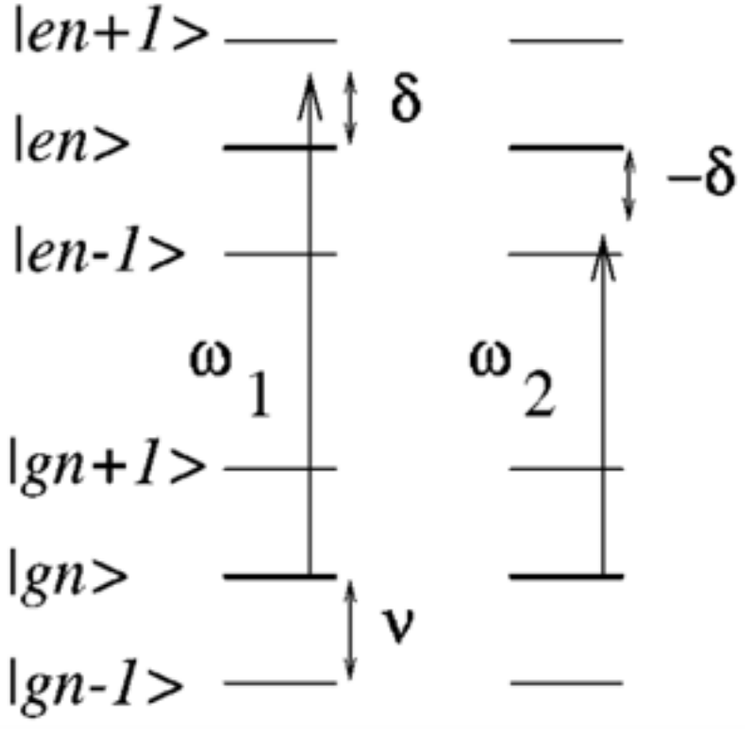


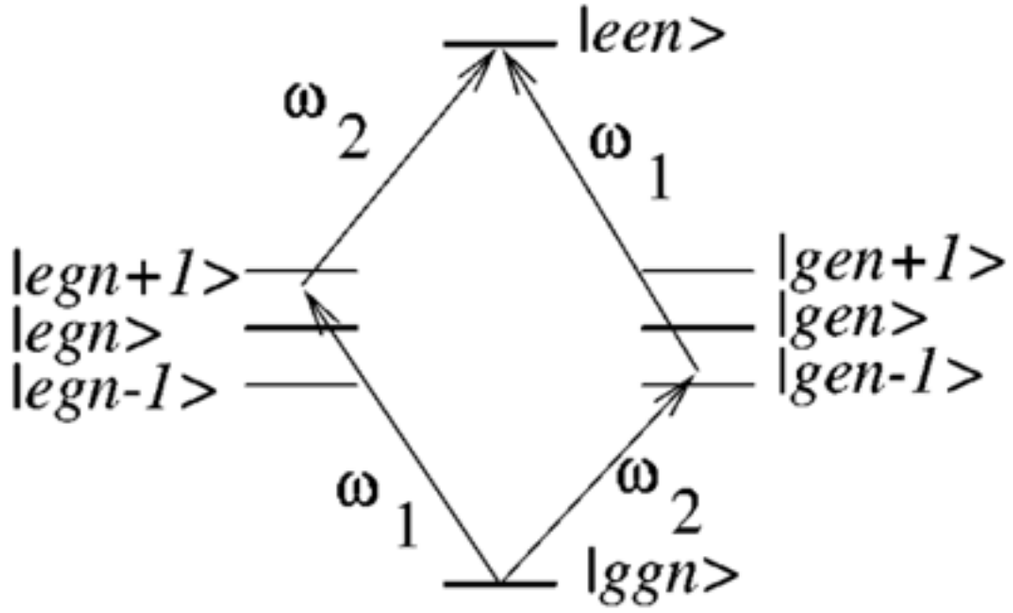
Molmer-Sorensen Gate

- Ion 1 and 2 are addressed with laser frequencies $\omega_{1/2} = \omega_0 \pm \delta$ respectively

- The laser setting couples the states
$|gg,n\rangle \leftrightarrow \{|eg,n+1\rangle, |ge,n-1\rangle\} \leftrightarrow |ee,n\rangle$

- The detuning from the sidebands are large enough so that the intermediate states $|eg,n+1\rangle$ and $|ge,n-1\rangle$ are not populated





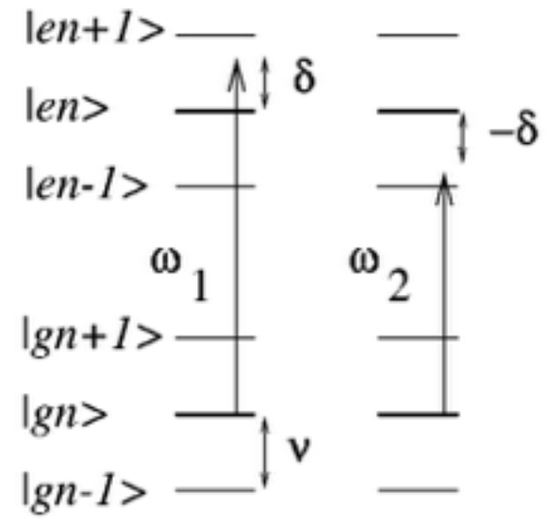
Molmer-Sorensen Gate

- The system can be described by the following Hamiltonian:

$$H = H_0 + H_{\text{int}},$$

$$H_0 = \hbar\nu(a^\dagger a + 1/2) + \hbar\omega_{eg}\sum \sigma_{zi}/2,$$

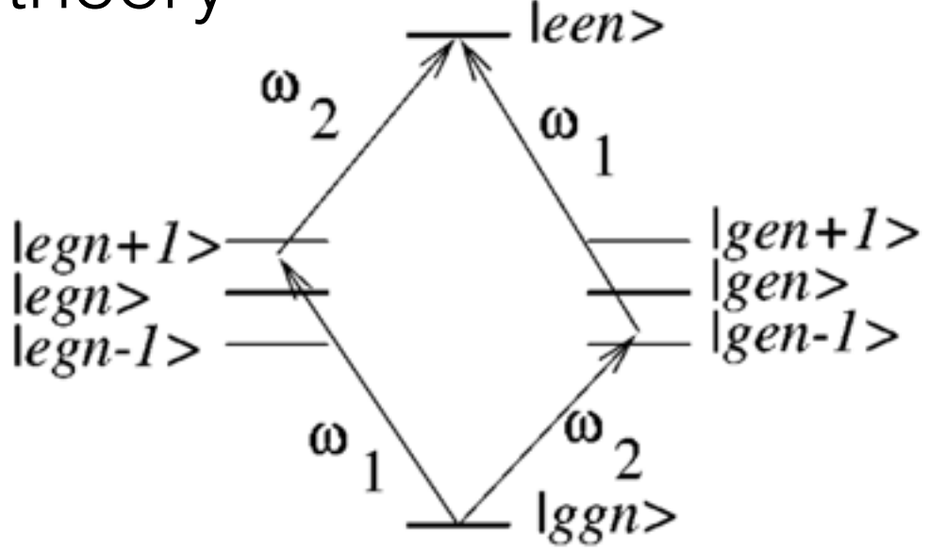
$$H_{\text{int}} = \sum_i \frac{\hbar\Omega_i}{2}\left(\sigma_{+i}e^{i[\eta_i(a+a^\dagger)-\omega_i t]} + \text{H.c.}\right),$$



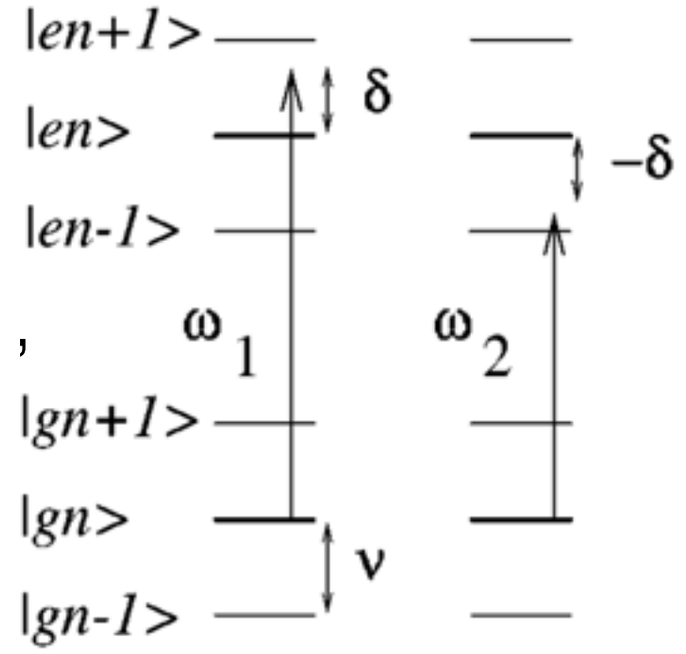
- The energy conserving transitions are between $|ee,n\rangle$ and $|gg,n\rangle$

- The Rabi frequency for the transition via states *m* can be determined in second order perturbation theory

$$\left(\frac{\tilde{\Omega}}{2}\right)^2 = \frac{1}{\hbar^2}\left|\sum_m \frac{\langle een|H_{\text{int}}|m\rangle\langle m|H_{\text{int}}|ggn\rangle}{E_{ggn} + \hbar\omega_i - E_m}\right|^2,$$



Molmer-Sorensen Gate



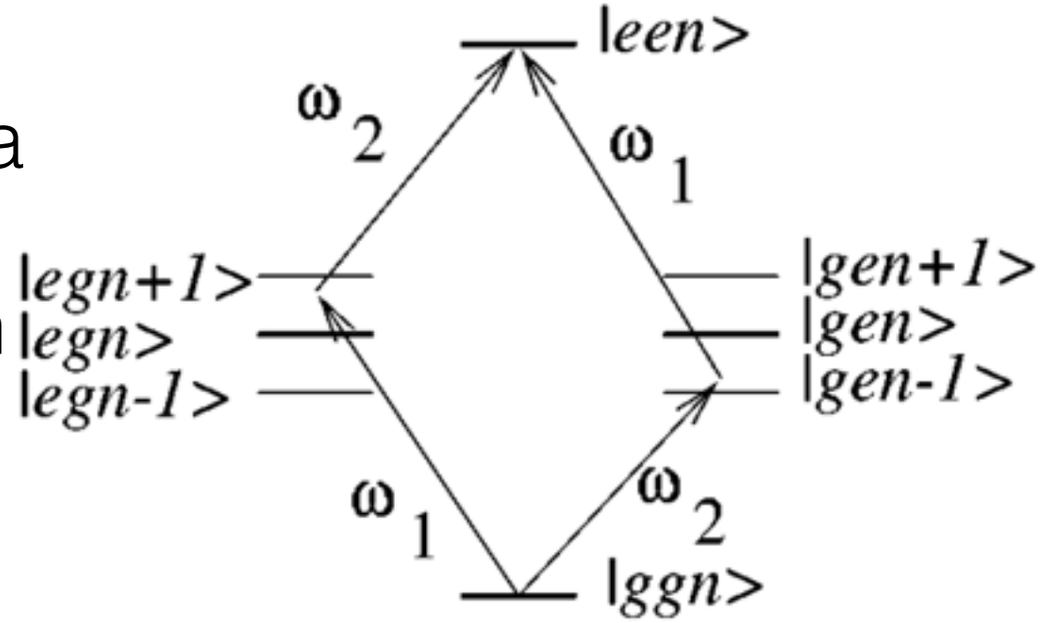
- If we restrict the sum to $|eg, n+1\rangle$ and $|ge, n-1\rangle$, we obtain the effective rabi frequency

$$\tilde{\Omega} = -\frac{(\Omega\,\eta)^2}{2(\nu - \delta)},$$

- No dependence on vibrational quantum number *n* due to interference between the two paths.

- The coherent evolution of the internal atomic state is thus insensitive to vibrational quantum numbers

- Evolution can be observed on ions in a superposition of vibrational states and even when heating of vibrational motion occurs



Molmer-Sorensen Gate

- Perturbations of the energy levels by the lasers will in general lead to decoherence effects

- To circumvent this, apply both frequencies to both ions

- Then there also exists resonant transitions between $|eg\rangle$ and $|ge\rangle$

- The MS gate then produces the following truth-table:

$$|gg\rangle \rightarrow \cos\left(\frac{\tilde{\Omega}T}{2}\right)|gg\rangle + i\sin\left(\frac{\tilde{\Omega}T}{2}\right)|ee\rangle,$$

$$|ee\rangle \rightarrow \cos\left(\frac{\tilde{\Omega}T}{2}\right)|ee\rangle + i\sin\left(\frac{\tilde{\Omega}T}{2}\right)|gg\rangle,$$

$$|ge\rangle \rightarrow \cos\left(\frac{\tilde{\Omega}T}{2}\right)|ge\rangle - i\sin\left(\frac{\tilde{\Omega}T}{2}\right)|eg\rangle,$$

$$|eg\rangle \rightarrow \cos\left(\frac{\tilde{\Omega}T}{2}\right)|eg\rangle - i\sin\left(\frac{\tilde{\Omega}T}{2}\right)|ge\rangle.$$

Digital Simulations

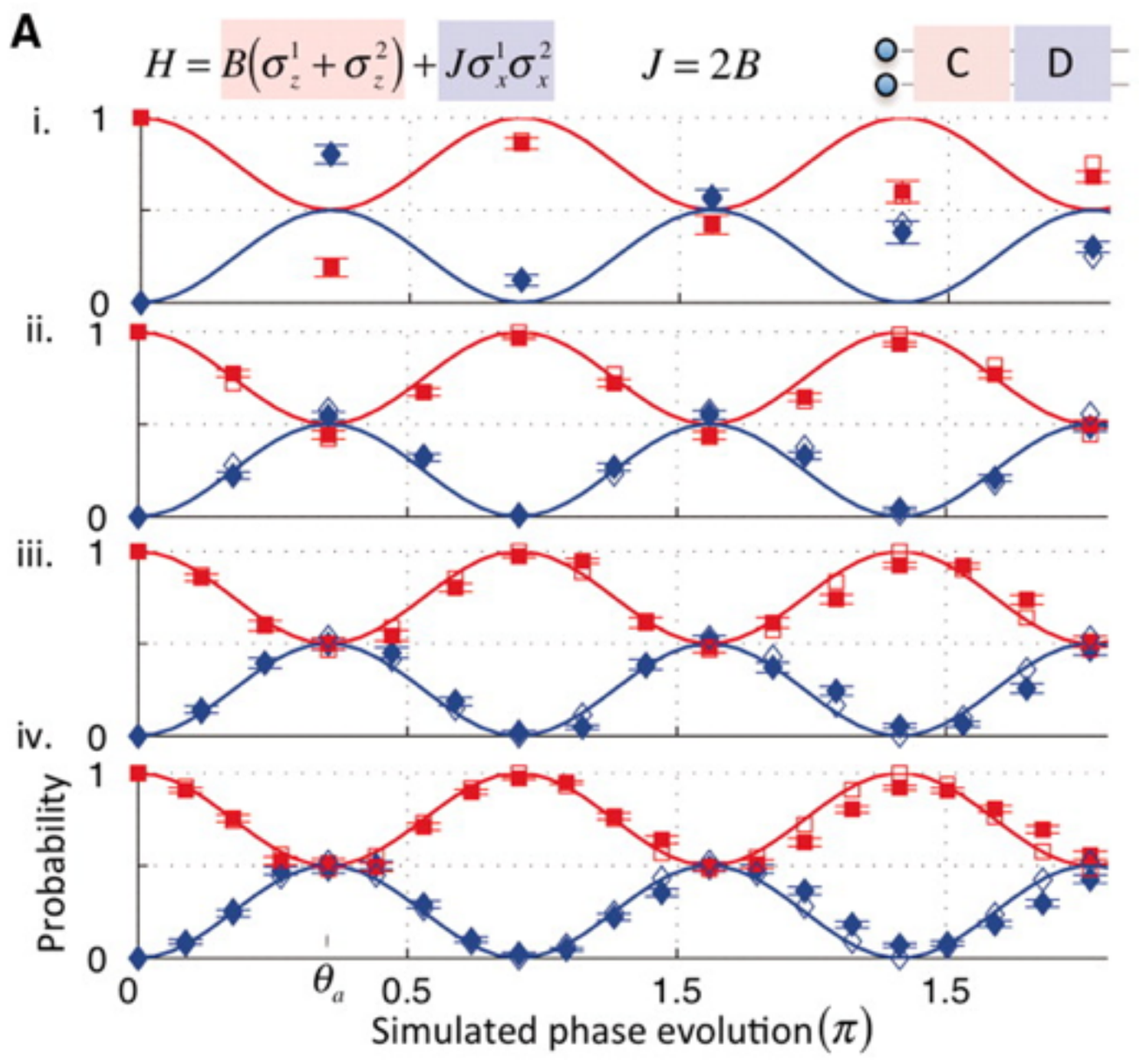
$$O_1(\theta, i) = e^{-i\,\theta\,\sigma_z^i}$$
$$O_2(\theta) = e^{-i\theta\,\Sigma_i\,\sigma_z^i}$$
$$O_3(\theta, \phi) = e^{-i\theta\,\Sigma_i\,\sigma_\phi^i}$$
$$O_4(\theta, \phi) = e^{-i\theta\,\Sigma_{i<j}\,\sigma_\phi^i\sigma_\phi^j}$$

2 spin time-independent Ising system

- Each digital step is
  $D.C = O_4(\theta_a/n, 0).O_2(\theta_a/2n)$
  where $\theta_a = \pi/2\sqrt{2}$ and
  n= 1,2,3,4 (i - iv respectively)

- Initial state is $|\uparrow\uparrow\rangle$

- Quantum process fidelities between simulation and exact dynamics (i) 61% and (iv) 91%



Lines show exact dynamics; ■ ↑↑ ◆ ↓↓

Digital Simulations

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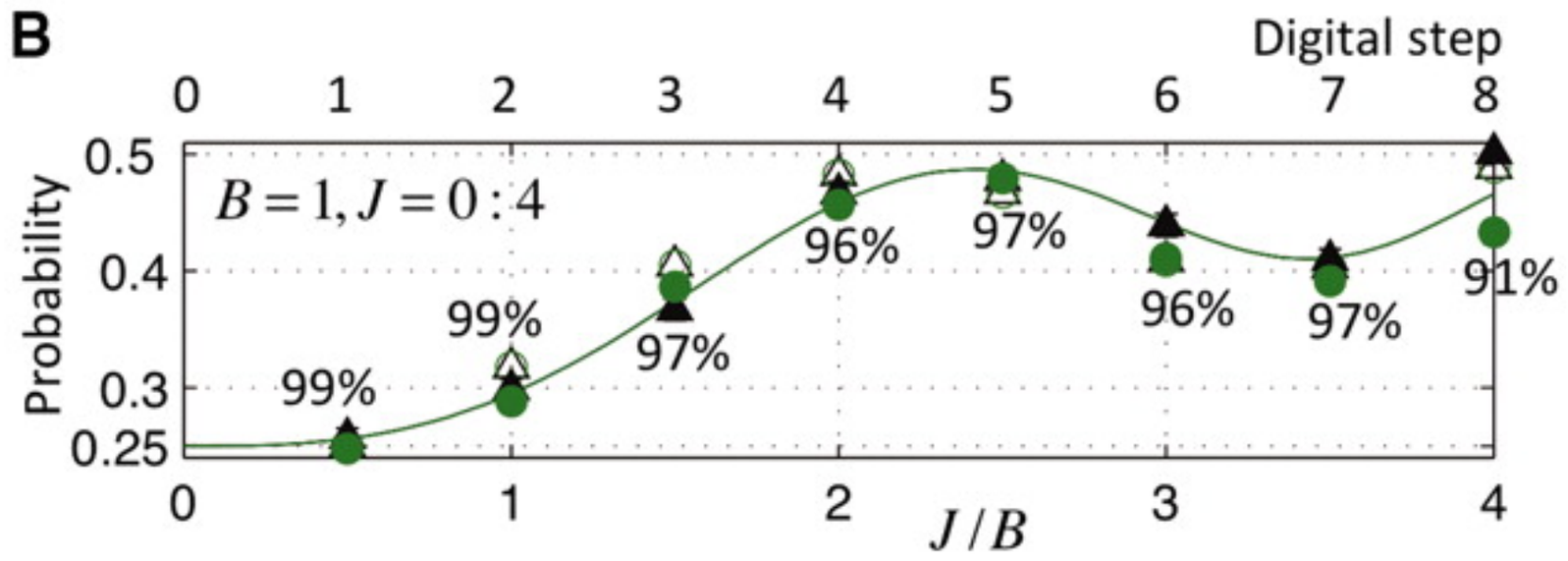
2 spin time-dependent Ising system

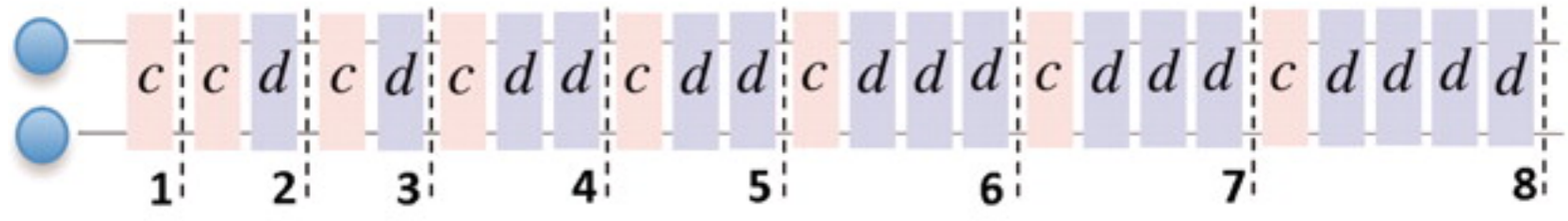
- J increases linearly from 0 to 4B

- Digitised linear ramp with $c = O_2(\pi/16)\ \ d = O_4(\pi/16, 0)$

- Initial state $|\uparrow\uparrow\rangle$



$$H = B\left(\sigma_z^1 + \sigma_z^2\right) + J\sigma_x^1\sigma_x^2$$



Lines show exact dynamics; unfilled shapes show ideal digitised;

■ ↑↑ ◆ ↓↓ ● $\rightarrow\rightarrow_X$ ▲ $\leftarrow\leftarrow_X$

Digital Simulations

$$O_1(\theta, i) = e^{-i\,\theta\,\sigma_z^i}$$
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$$O_3(\theta, \phi) = e^{-i\theta\,\Sigma_i\,\sigma_\phi^i}$$
$$O_4(\theta, \phi) = e^{-i\theta\,\Sigma_{i<j}\,\sigma_\phi^i\sigma_\phi^j}$$

Ising, XY and XYZ Model

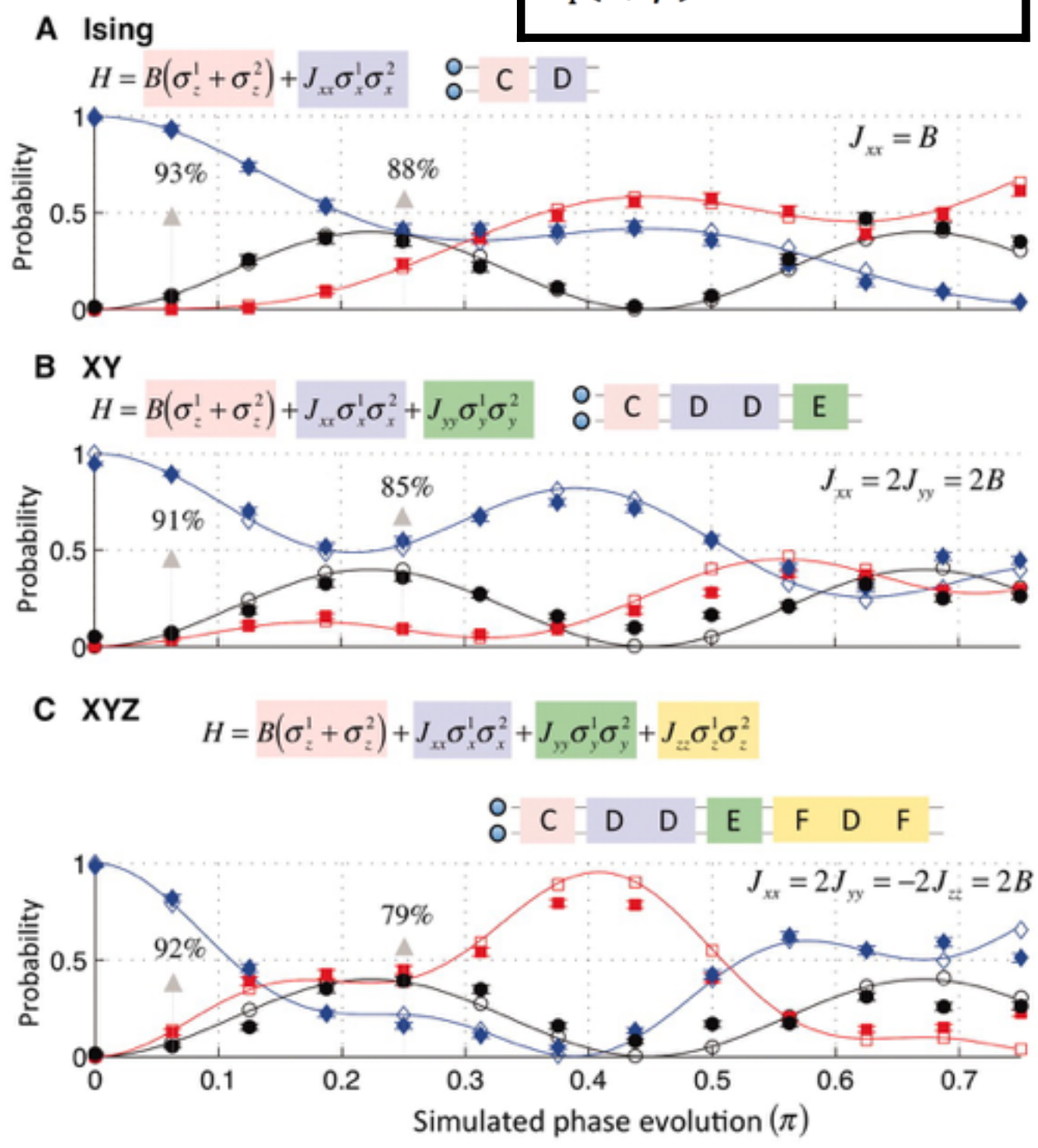
- Initial state $|{\rightarrow\leftarrow}\rangle_x$

- Fixed digital resolution of $\pi/16$ with 12 Trotter steps

- Show close agreement with exact dynamics

- Fidelities: 88%, 85%, 79% respectively

$$C = O_2(\pi/16) \quad D = O_4(\pi/16, 0)$$
$$E = O_4(\pi/16, \pi/2) \quad F = O_3(\pi/4, 0)$$



Lines show exact dynamics; unfilled shapes show ideal digitised; ■ $\uparrow\uparrow$ ◆ $\downarrow\downarrow$ ● $\rightarrow\rightarrow_x$ ▲ $\leftarrow\leftarrow_x$

Digital Simulations

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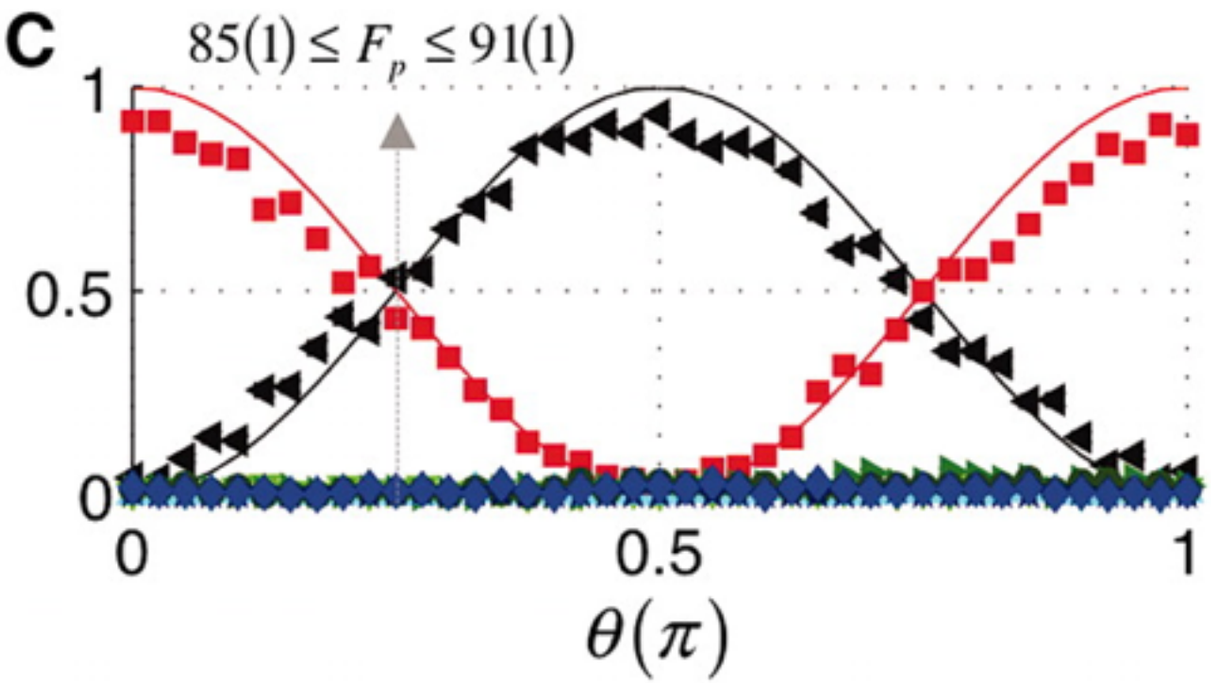
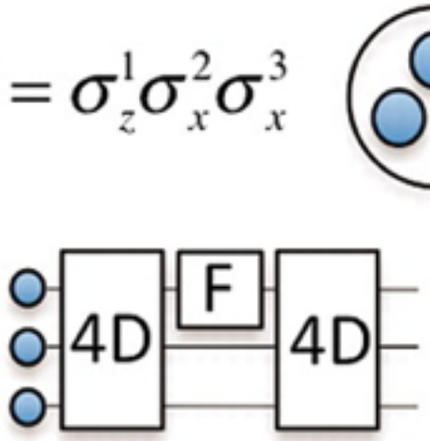
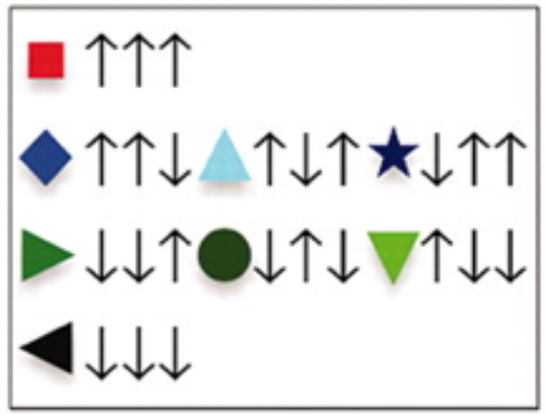
$$O_4(\theta, \phi) = e^{-i\theta\,\Sigma_{i<j}\,\sigma_\phi^i\sigma_\phi^j}$$

3-body interaction

$$4D = O_4(\pi/4, 0)$$
$$F = O_1(\theta, 1)$$
$$H = \sigma_z^1\sigma_x^2\sigma_x^3$$







Lines show exact dynamics

- there exists circuit decompositions involving one and two qubit gates that can simulate many-body interactions

- the measurements were taken after a rotation into the logical σ_z basis

- initial state is the $|{\rightarrow}{\rightarrow}{\rightarrow}\rangle_y$ state

Digital Simulations

$$O_1(\theta, i) = e^{-i\,\theta\,\sigma_z^i}$$
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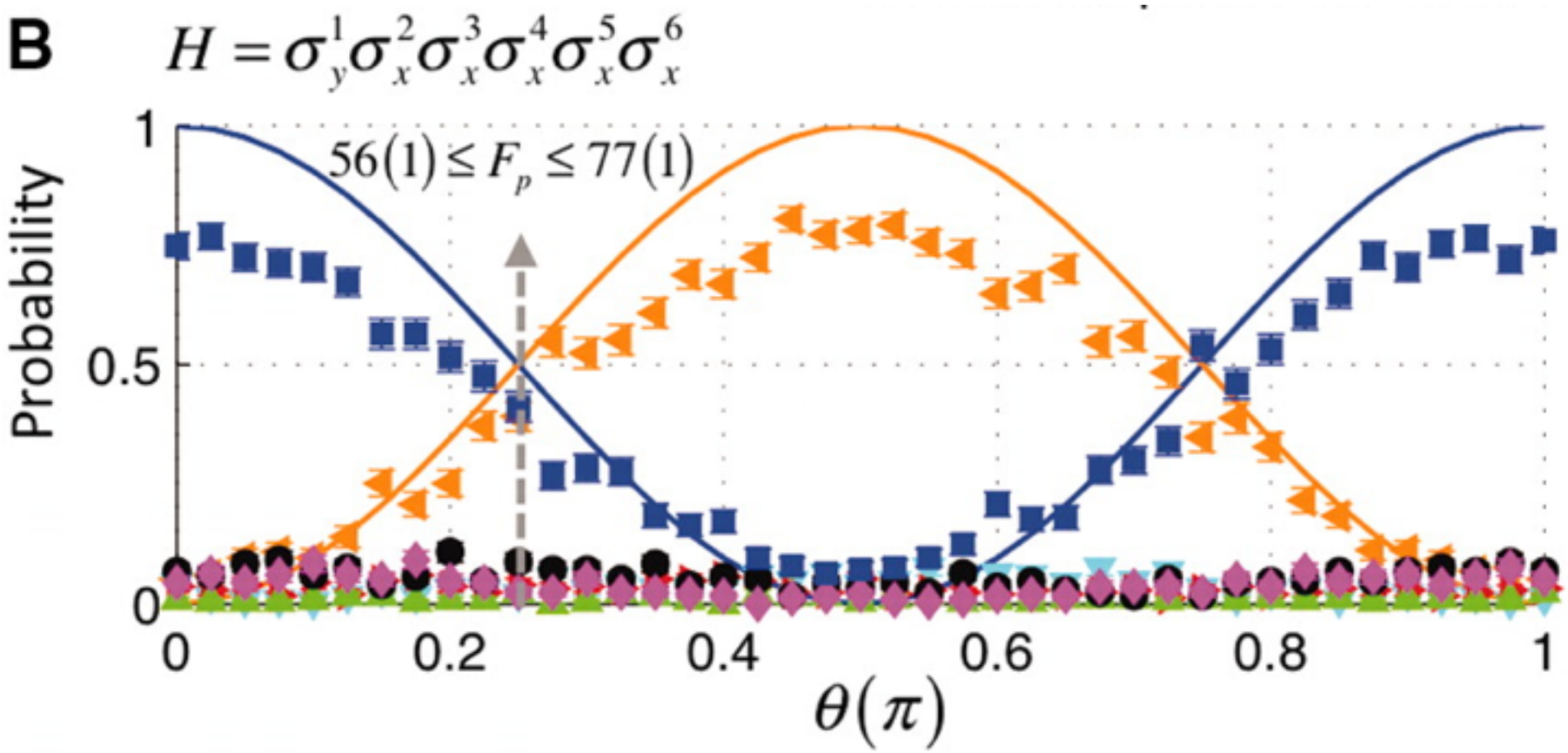
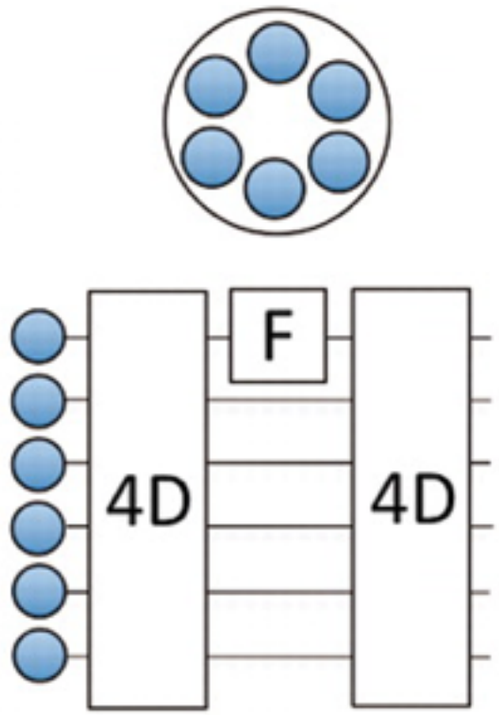
$$O_4(\theta, \phi) = e^{-i\theta\,\Sigma_{i<j}\,\sigma_\phi^i\sigma_\phi^j}$$

6-body interaction

$$4D = O_4(\pi/4, 0)$$
$$F = O_1(\theta, 1)$$





Lines show exact dynamics; P_i is the probability of finding i spins pointing down

Conclusion

- The leading source of error which dominates the decoherence process is laser intensity fluctuations

- This is not a fundamental limitation and can potentially be improved to increase simulation capabilities

- Have provided evidence that the level of control required for a full-scale device is within reach

- Further work needs to be done to scale up the processes for a full-scale device but it remains a promising outlook for the future

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