Fast Gates Allow Large-Scale Quantum Simulation with Trapped Ions

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Ion traps are a promising platform for the implementation of various quantum technologies, particularly quantum simulation. Unfortunately, the entangling gates required for digital quantum simulations rely on the virtual excitation of the motional modes of the trap, making the necessary operations too slow with respect to the system coherence times. In this work, we propose a method of implementing a crucial multiqubit gate, through a scheme of fast two-qubit gates, able to perform in shorter time and with more precision than existing alternatives. Its implementation would enable digital quantum simulations to outperform classical computers without error correction.

Quantum simulations promise the ability to study the dynamics of highly complex quantum systems using more easily accessible and controllable systems [1–3]. Digital quantum simulation schemes, using quantum computing resources, enable versatile simulations of a collection of systems - indeed, a universal set of quantum gates is sufficient to compose any desired unitary arising from a local Hamiltonian [4]. This compares to analogue quantum simulation schemes that require precise engineering of a Hamiltonian to reproduce the desired dynamics of the simulated system [3]. Analogue simulations require a direct mapping between the simulator and system Hamiltonians, and are necessarily less versatile than digital quantum simulations. Moreover, the latter, due to their similarities with gate-based quantum computing schemes, may allow for error correction.

Many systems are considered as potential quantum simulators [3]: cold atoms in optical lattices [5], superconducting circuits [6], and nuclear spin systems [7, 8], in addition to trapped ions [9, 10]. Each simulator platform has its own advantages and challenges - cold atoms scale well but are difficult to control individually, whereas trapped ions and superconducting circuits face scaling difficulties but have experimentally-demonstrated individual control and readout techniques [11]. Concerning the possibility of implementing digital quantum simulations, trapped ions [12–16] and superconducting circuits [17–19] have demonstrated a great potential. In particular, implementations in ion traps, involving interacting spins and fermions, rely on the efficient and high-fidelity implementation of Mølmer-Sørensen (MS) gates [20] along a specific operation sequence,

$$U_{\mathrm{MS}}^{\dagger}\left(\frac{\pi}{2}\right) U_{\sigma_z^m} U_{\mathrm{MS}}\left(\frac{\pi}{2}\right). \tag{1}$$

Here, $U_{\mathrm{MS}}(\frac{\pi}{2})$ is an MS gate and $U_{\sigma_z^m}$ is a local rotation on the mth ion in the trap. The MS gate couples every pair of ions in the trap evenly,

$$U_{\mathrm{MS}}(\theta) = e^{-i\frac{\theta}{4}\sum_{k,l=1}^{L}\sigma_x^k\sigma_x^l}, \tag{2}$$

where σ_x^k is the Pauli x operator on ion k, and L the total number of ions. These gates can be implemented with reasonable fidelity in ion traps [21, 22], but are slower than the trap period due to their reliance on the Lamb-Dicke regime and the vibrational rotating-wave approximation. This means it would be difficult to use MS gates for a quantum simulation of a sufficient size, say dozens of interacting spins or fermions, to outperform classical computers. Though MS gates become too slow with scaling, in Eq. (1), each MS gate can be replaced by an ultrafast multiqubit gate (UMQ) [16],

$$U_{\mathrm{UMQ}} = e^{-i\frac{\pi}{4}\sigma_x^m\sum_{k=1,k\neq m}^{L}\sigma_x^k}, \tag{3}$$

coupling only pairs involving the locally-rotated ion.

In this Letter, we propose and analyze the replacement of the MS gate in trapped-ion digital quantum simulation schemes [12–16] by an implementation of the UMQ gate using fast two-body gates performed by ultrafast laser pulses [23–31]. We perform analytical and numerical simulations to validate our approach, and find that it may be feasible with current or near-future technology. This will allow us to overcome the time barrier imposed by the MS gate and significantly reduce the operation time of digital quantum simulations, as well as greatly increase the final fidelity. The latter implies that large-scale quantum simulations could be performed without error correction, permitting to solve problems in condensed matter, quantum chemistry, and high-energy physics, which are infeasible to classical computers.

Fast two-qubit gates can be performed beyond the trap-period limit and implement the ideal unitary for a geometric phase gate,

$$U_{\mathrm{I}} = e^{i\frac{\pi}{4}\sigma_z^1\sigma_z^2}, \tag{4}$$

where σ_z^k is the Pauli z operator on the kth ion. These gates are implemented using counter-propagating laser π-pulse pairs, which act as state-dependent momentum kicks on the motional modes while preserving the internal states of the ions. This behaviour is described in the optical rotating-wave approximation by the kick unitary

$$U_{\text{kick}} = e^{-2izk(x_1\sigma_z^1 + x_2\sigma_z^2)}. \tag{5}$$

Here, x_c is the position operator on ion c, z is the number of π-pulse pairs used for the momentum kick and k is the laser wavenumber. These kicks are nearly instantaneous compared to the trap period, so the evolution of a real gate operation can be expressed as the product of the kick unitaries interspersed with free motional evolution,

$$U_{\text{re}} = \prod_{c=1}^{N} \left(\prod_{p=1}^{L} e^{-i\nu_p a_p^\dagger a_p \delta t_c} \right) U_c, \tag{6}$$

where U_c is the cth kick unitary, δt_c is the time between kicks c and $c+1$ (0 if $c = N$) and N is the total number of kicks. An analytic solution for this evolution to implement the ideal unitary in Eq. (4) cannot generally be found, so numerical methods are used to optimise the fidelity of the resulting gate. The high-fidelity solutions found by this optimisation approach will restore the initial motional state of the trap, while the state-dependent phase-space trajectories for the motional modes will enclose areas corresponding to the $\frac{\pi}{4}$ phase required by the ideal unitary. This results in a geometric phase gate that produces minimal trap heating.

The structure of the kicks is chosen to be antisymmetric, which approximately restores the motional state - the dominant motional error term is cubic with respect to gate time [24]. This reduces the difficulty of the numerical optimisation and produces generally higher-fidelity solutions. In particular, the Fast Robust Antisymmetric Gate (FRAG) scheme [29] was found to give the shortest gate times for a target fidelity using realistic experimental parameters. This scheme uses the kick sequence

$$\begin{aligned} z = (&-n, & 2n, & -2n, & 2n, & -2n, & n), \\ t = (&-\tau_1, & -\tau_2, & -\tau_3, & \tau_3, & \tau_2, & \tau_1), \end{aligned} \tag{7}$$

where z is the set of kick magnitudes associated with the times t, n is an integer and $\tau_1 > \tau_2 > \tau_3 > 0$. A negative kick magnitude indicates a kick in the opposite direction. The fast gates used for our analysis in this work are based on the FRAG scheme, but with the restriction on kick ordering removed. This preserves the antisymmetric structure of the sequence, but gives numerical optimisations access to a larger parameter space, yielding higher-fidelity gate solutions in many cases. We also address the transverse motional modes of the trap, which act analogously to the longitudinal modes [32] but allow easier addressing of individual ions.

We can use fast geometric phase gates to implement the UMQ gates required in digital quantum simulations. If we label the ions in a Paul trap from 1 to L starting at one end, this is done by performing a fast gate on ions 1 and 2, a swap gate on these ions, then a fast gate on ions 2 and 3 and so on until we reach ions $L-1$ and L. This gives the UMQ unitary required up to local rotations, not preserving the position of the internal states in the trap. The reversed UMQ gate in the simulation step restores the position of the internal states. It should be noted that this method of constructing a UMQ gate requires fast swap gates, which can be implemented with three CNOT gates [33]. Each CNOT requires one fast geometric phase gate and some local rotations.

This allows us to implement a non-position-preserving UMQ gate using $L-2$ swap gates and an additional $L-1$ fast gates, for a total of $4L-7$ fast gates. Due to the relative timescales and fidelities of local rotations, which require only single laser pulses that take negligible time and can be performed with very high fidelity [34], we consider only infidelity and time cost of the fast two-qubit gates in our results. We estimated fidelities for a UMQ gate by first calculating the fidelities of the component two-qubit gates. This calculation was performed with a state-averaged fidelity measure, assuming an initial thermal product state for the motional modes of the trap. This fidelity measure is given by

$$F = \frac{\int_{\psi_0} \text{Tr}_m [\langle\psi_0| U_{\text{id}}^\dagger U_{\text{re}} |\psi_0\rangle \langle\psi_0| \otimes \rho_m U_{\text{re}}^\dagger U_{\text{id}} |\psi_0\rangle] \mathrm{d}\,|\psi_0\rangle}{\int_{\psi_0} \mathrm{d}\,|\psi_0\rangle}, \tag{8}$$

where U_{re} and U_{id} are the real and ideal gate operations, respectively. The assumption of a thermal product state simplifies expectation values of motional displacement operators that appear upon expanding this expression, allowing the calculation of an analytic expression for the state-averaged fidelity given a set of kick times. This expression simplifies numerical optimisation by removing the need to calculate the full unitary U_{re}.

We optimised this fidelity for every adjacent pair of ions in Paul traps of various sizes. The longitudinal trap frequency was chosen as $\nu = 2.1856$ MHz $\times L^{-0.865}$, where the power of L represents a no-buckling limit for the trap derived from molecular dynamics simulations [35, 36] and the constant coefficient is chosen to give a typical trapping frequency of 1.2 MHz for a two-ion trap. The transverse trap frequency was constant at $\nu_x = 5$ MHz. The Lamb-Dicke parameter was $\eta = 0.16$ for the two-ion trap, and scaled appropriately with trapping frequency for larger traps [21].

The results of this optimisation are shown in Fig. (1). An estimate of total fidelity for the UMQ gate on the trap is obtained by multiplying the fidelities of all the constituent fast gates. This should give a lower bound on the true UMQ fidelity, as this method assumes gate
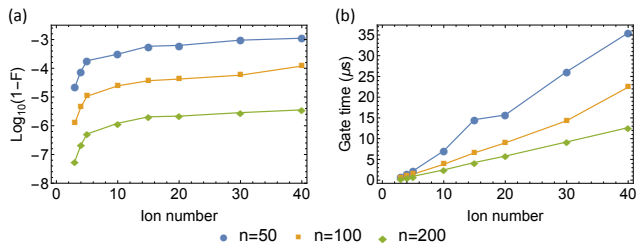
FIG. 1. Plots of (a) fidelity and (b) gate time for UMQ gates implemented with fast gates on traps of varying sizes. n represents the number of π-pulse pairs used for each momentum kick. The initial motional state is a thermal state with average occupation $\bar{n} = 0.1$ for each mode.

errors are perfectly correlated. We see that the fidelity achieved by the numerical optimisation decays with the size of the trap, which is expected because more motional modes must be restored to their initial state while contributing to an ideal phase for the gate. However, we do see very high fidelity overall, even for larger traps. The $n = 100$ fast gate, corresponding to a minimum laser repetition rate of around 30 GHz, achieves a UMQ gate fidelity of 99.988% in a 40-ion trap. This would correspond to fidelity of around 70%, without including error correction, for 10 Trotter steps of a 20-site fermionic lattice simulation, requiring 2680 UMQ gates.

In Fig. (1b), we analyze the dependence on time of our fast gates scheme. Again focusing on the $n = 100$ case, the time required for a 40-ion UMQ gate is 22.4 µs, comparable with the trap period of 10 µs for this trap. Further to this, the trap period does not place any fundamental limit on the speed of fast gates as it does with MS gates. In general, an MS gate for N ions will take a time $\sqrt{N}t_1$, t_1 being the time it takes for 1 ion. This can be seen from the expression of the gate's phase in terms of experimental parameters, $\theta \propto (\frac{\Omega\eta}{\delta})^2$. Here Ω is the Rabi frequency, which does not depend on the number of ions and is limited by the laser power, η is the Lamb-Dicke parameter, which for N ions is given by $\eta_1/\sqrt{N}$, where η_1 is the single-ion Lamb-Dicke parameter, when the COM vibrational mode is considered. The detuning δ sets the gate time to $t = 1/\delta$. It is clear that to compensate for the $1/N$ decay rate of θ with the number of ions, the detuning has to be decreased accordingly, $\delta \to \delta/\sqrt{N}$, which increases the time of the MS gate as $t \to \sqrt{N}t$. A two-qubit MS gate is typically around 50 µs long [21], showing that a 40-ion gate would take an order of magnitude more time than our UMQ gate implementation.

There is a clear trend towards higher fidelity and lower gate time with higher momentum in the results shown in Fig. (1b), which means the development of faster pulsed lasers would lead to an even more favourable comparison with the MS gate. We have shown that under ideal conditions, a very high-fidelity UMQ gate can be performed

using fast gates. However, to consider the experimental feasibility of performing simulations of interacting spins and fermions using fast gates, we should analyse the effects of potential sources of error on the gates. In particular, errors in π pulse area have been shown to affect gate fidelity significantly [29]. We will also consider dynamical effects of decoherence during the gate evolution.

To consider the effect of an error in π pulse area on a gate applied to an adjacent pair of ions in a large trap, we employed a method relying on the assumption that the motional mode dynamics are separable during the gate, a valid assumption for small π pulse errors in harmonic trapping potentials. This enables computationally feasible simulation of the gate evolution, allowing simple calculation of a representative-state fidelity for various levels of π pulse error [37]. The initial motional state is chosen as the first excited number state for each motional mode, allowing simulations with state vectors. The representative-state fidelity is

$$F = \left| \langle \psi_0 | U_{re}^\dagger U_{id} | \psi_0 \rangle \right|^2, \tag{9}$$

where $|\psi_0\rangle$ is the state $\frac{1}{\sqrt{2}}(|00\rangle + |01\rangle)$, chosen to give an even superposition of the two-qubit computational basis states - the gate's action is identical if the qubits are flipped, even with imperfect pulses, so $|10\rangle$ and $|11\rangle$ are not necessary in the superposition.
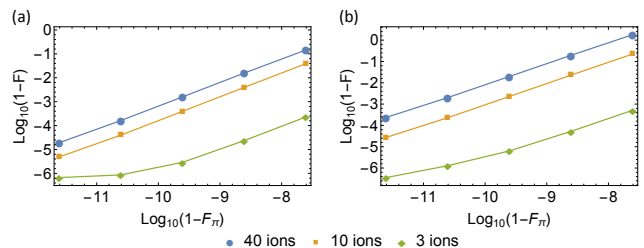

FIG. 2. A plot of infidelity for (a) a two-qubit $n = 100$ fast gate and (b) a full UMQ gate against the rotational infidelity in each π pulse, F_π. The error in (b) is estimated assuming the errors in successive fast gates are uncorrelated.

We simulated two-qubit fast gates on the outermost adjacent pair of ions (ions 1 and 2) in traps of varying size. The results of these simulations are shown in Fig. (2a). Simulations used square pulses with a Rabi frequency given by $\Omega = \frac{\xi\pi}{2\tau}$, where τ is the pulse time such that $\xi = 1$ gives a perfect π pulse. Results are plotted against rotational infidelity $1 - F_\pi$, where $F_\pi = \left| \langle \psi_0 | U_{\pi re}^\dagger U_{\pi id} | \psi_0 \rangle \right|^2$, and $U_{\pi re,id}$ are the real and ideal unitaries for the π pulse. For this square pulse this rotational infidelity is approximately $\frac{\pi^2}{4}(1 - \xi)^2$ [37–39].

We also simulated a full UMQ gate on a three-ion trap with low-momentum fast gates and imperfect π pulses. Comparing the infidelity of the entire UMQ operation to

that of a single fast gate with the same π pulse imperfection, it was determined that errors due to π pulse imperfections in successive fast gates are uncorrelated, and thus this type of error scales with the number of gates applied as $\sqrt{N}$. This allowed estimation of the error for a complete UMQ gate with imperfect π pulses, shown in Fig. (2b). Given this estimation, for rotational infidelity over 10^{-11}, the gate infidelity is too high to implement a 40-ion simulation with an estimated fidelity above 50%. Thus, we can place this limit on π pulse errors for fast gates to be useful for a quantum simulation outperforming classical computers without error correction. Proposals exist for composite pulse schemes which can produce extremely high fidelities, robust to the type of intensity instability or miscalibration that would damage a square pulse [38]. Analysis of such composite schemes shows that they are also useful for sub-diffraction-limited addressing of ions in a densely-populated trap [39], another factor that could influence fidelity.

We also considered the effect of decoherence during fast gate evolution, in order to place a limit on the rate of decoherence processes to maintain the high fidelity of fast gates. In this case, a full simulation is not feasible for a 40-ion trap, so our results are inferred from simulations of decoherence effects on a low-momentum ($n = 2$) fast gate on a two-ion trap. The full evolution of this gate was simulated, assuming the momentum kicks to be approximately instantaneous and thus unitary, and solving a master equation using a Monte Carlo trajectory approach during the free evolution periods of the gate.

We simulated the effects of trap heating and dephasing separately. The state of the trap evolves in the absence of laser light according to the master equations

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \Gamma_{\mathrm{h}} \sum_p (\mathcal{D}[a_p] + \mathcal{D}[a_p^\dagger])\rho, \qquad (10)$$

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \Gamma_{\mathrm{d}} \sum_k \mathcal{D}[\sigma_z^k]\rho. \qquad (11)$$

Here, Γ_{h} and Γ_{d} are trap heating and dephasing rates, respectively, while $\sum_p$ represents a sum over motional modes and $\sum_k$ a sum over ions. Here, $\mathcal{D}[O]\rho \equiv O\rho O^\dagger - \frac{1}{2}(O^\dagger O\rho + \rho O^\dagger O)$, and the Hamiltonian is given by $H = \sum_p \hbar \nu_p a_p^\dagger a_p$. We have assumed an infinite temperature reservoir for trap heating, a valid model for a randomly fluctuating electromagnetic field [11]. Fidelity is again calculated using a representative state starting in the motional ground state. We trace out the motional state to calculate the computational fidelity after decoherence has been included in the simulations.

The results of these simulations are shown in Fig. 3. The infidelity calculated under trap heating shows that heating during gate evolution has a dynamical effect on the gate, damaging the phase accumulation required to implement the ideal unitary. The fidelities shown here
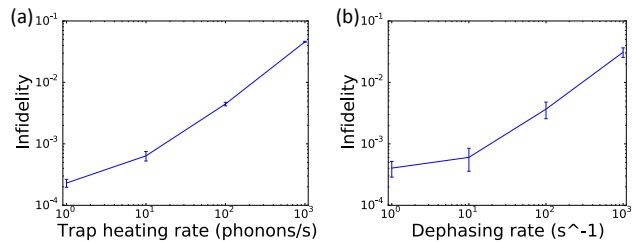

FIG. 3. Infidelity of an $n = 2$ two-qubit fast gate in a two-ion trap under (a) trap heating and (b) dephasing.

are lower than that of a gate acting on a hotter initial state, meaning that the decoherence must be affecting the evolution of the gate. This can be understood physically as the heating changing the motional phase space trajectory of the gate. The effect of dephasing is similar to that of trap heating. The physical reasoning behind dephasing affecting the gate is more obvious, as dephasing directly affects the phase of the state.

We can extend the conclusions drawn from these results to larger traps. If phonon absorption significantly damages the gate, we must work in a regime where a phonon absorption is quite unlikely during any operation. Considering that our 40-ion simulation would take around 3 ms, this limits both dephasing and heating rates to below 100 s^{-1} for a high-fidelity simulation [11].

Fast gates have been proposed as a superior two-body gate for trapped ion quantum information processing, being much faster than existing gates and robust to many sources of error. In this work, we have analysed the potential for fast gates to implement useful digital quantum simulations, enough to outperform a classical computer. We have also studied the limits on experimental apparatus to successfully implement high-fidelity operations using fast gates. High-performing gates require rotational fidelities on the order of 10^{-11} and decoherence rates below 100 s^{-1}. If these requirements are satisfied, it appears that fast gates can significantly outperform MS gates in terms of gate time, and can be implemented with very high fidelity if high-repetition-rate lasers are available [40]. Therefore, fast gates hold significant promise for the future of trapped ion quantum simulation and quantum information processing.

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