## Numerical simulation of the performance of single qubit gates for trapped ions

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Quantum computing with trapped ions has shown significant progress over the last couple of decades [1– 5]. The main advantages are the highest-fidelity quantum computing gates, long coherence times, inherent uni-formality and all-to-all connectivity [6–11]. Nowadays the attention has shifted from miniature architectures towards more practical implementations requiring to scale up the computer performance [12–19]. For large ion crystals system performance is known to degrade [1]. Therefore, it is crucial to understand scaling of the finite errors in quantum gates with the system size due to noise, decoherence, and control imperfections. In particular, we numerically studied the performance of global single-qubit gates depending on the Lamb-Dicke parameter, gate time, the number of ions, and the initial phonon mode occupation numbers.

The dynamics of single-qubit gates in trapped-ion systems is typically described using Lamb–Dicke approximation meaning the exclusion of the phonon modes [2, 7, 20]. In this work we performed numerical simulation of the action of the single qubit gate  $R_{\phi}(\theta)$  using full Hamiltonian of the system (1):

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$$\hat{H}_N = \sum_{p=1}^N \hbar \frac{\omega_q}{2} \hat{\sigma}_z^p + \sum_j \sum_{k=1}^N \hbar \omega_{jk} \left( \hat{a}_{jk}^{\dagger} \hat{a}_{jk} + \frac{1}{2} \right) + \frac{\hbar}{2} \sum_{p=1}^N \Omega \left[ e^{-i(\omega t - \mathbf{k} \hat{\mathbf{R}}_p + \phi)} \sigma_p^+ + \text{h.c.} \right].$$
(1)

Here indexes p and j refer to the ion index in the chain and to the choise of the Cartesian axis (x, y, z) respectively,  $\omega_q$  is the qubit transition frequency,  $\omega$  is the laser frequency,  $\omega_{jk}$  is the frequency of the normal mode kalong axis j,  $\hat{a}_{jk}^{\dagger}/\hat{a}_{jk}$  are creation/annihilation operators of the normal mode k along axis j,  $\mathbf{k}$  is the wave vector of the laser,  $\phi$  is the phase of the laser, and angle  $\theta = \tau \Omega$  of the gate is controlled via the gate time  $\tau$ ,  $\hat{\mathbf{R}}_p$  is the quantised coordinate of the center of mass of

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ion p. Full Hamiltonian allows to account for the two effects responsible for gate errors: entanglement between the qubit states and the phonon modes and phonon mode heating which leads to the finite occupation of the phonon modes.

The results are obtained for optical Ca qubits and for the two types of gates,  $G_1$  and  $G_{15}$  for which the  $\pi/2$  pulse is performed during 1 s and 15 s, respectively [7, 2]. Figure 1 shows the fidelity of single-qubit  $R_{\phi}(\theta)$ gate for 3 ions for gates  $G_1$  and  $G_{15}$  with different levels of corrections to the Rabi frequency obtained in the Lamb-Dicke approximations (for details see [21]):

$$\Omega_p = \Omega\left(1 - \sum_j \sum_{k=1}^N \eta_{pjk}^2 (n_{kj} + 1/2)\right).$$
 (2)

The corrected Rabi frequencies  $\Omega$  account only for the finite occupation of the phonon modes. According to Fig. 1, the minimum infidelity of  $10^{-4}$  is achieved for the gate  $G_{15}$ , when the corrections for all the modes are included. Additional simulations indeed have shown that the phonon mode occupation leads to a more rapid decrease in the fidelity. For the fast  $G_1$  gate the situation is worse: the oscillations of fidelity can not be removed by correcting Rabi frequency. These oscillations come from the entanglement between the phonon modes and the qubit states. Comparison of the two different types of fidelities (obtained with and without tracing of the phonon modes) and calculations of the entanglement entropy also show the existence of entanglement between phonons and ions. The amplitude of the fidelity oscillations scales with  $\Omega$  and increases with the phonon mode occupation number. The largest contribution to the infidelity and to the amplitude of its oscillations comes from the population of the center of mass (COM) mode. We also studied the dependence of the fidelity on the Lamb-Dicke parameter and on the number of ions (from 1 to 4) for the initial phonon mode state  $|100\rangle$  corresponding to a single phonon in a COM mode. We observe less

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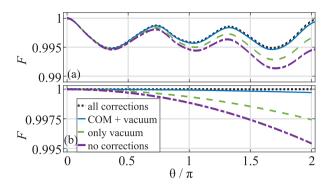


Fig. 1. (Color online) Computed fidelities of the singlequbit gates  $G_1$  (top panel) and  $G_{15}$  (bottom panel) depending on angle  $\theta$ . The initial state of phonon modes is  $|n_{\rm COM}n_2n_3\rangle = |211\rangle$ . Different line styles distinguish different cases depending on how the ideal gate operation was simulated: using corrections for the Rabi frequency (the colored lines except the dashed-dotted one) from Eq. (2) or without the corrections (dashed-dotted line). The number of modes/phonons accounted for the corrections is specified in the legend

profound decrease of the fidelity as the ion chain gets longer and for the larger axial frequencies.

In summary, the gate fidelities improve for slower gates and small Lamb-Dicke parameter n. For slow gates, the gate performance can be well characterised with modified Rabi frequency using Eq. (2), whereas for gates as fast as  $G_1$  numerical simulations are required to account for the entanglement effects and oscillatory behaviour of gate fidelity which originates from the ionphonon entanglement. Its period and amplitude scale with the Rabi frequency  $\Omega$ , the Lamb–Dicke parameter  $\eta$  and the phonon mode occupation number. The developed software package will be used to optimise singlequbit gate parameters for experimental setup handling trapped ions. The results and analyses will be useful for error mitigation in quantum algorithms performed on ions, optimisation of long gate sequences as well as the development of new variational algorithms accounting for present error models.

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