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High-fidelity ion-trap quantum computing with hyperfine clock states

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We propose the implementation of a geometric-phase gate on magnetic-field-insensitive qubits with $\hat{\sigma}^z$-dependent forces for trapped ion quantum computing. The force is exerted by two laser beams in a Raman configuration. Qubit-state dependency is achieved by a small frequency detuning from the virtually excited state. Ion species with excited states of long radiative lifetimes are used to reduce the chance of a spontaneous photon emission to less than 10^{-8} per gate run. This eliminates the main source of gate infidelity in previous implementations. With this scheme it seems possible to reach the fault-tolerant threshold.

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One of the big challenges in quantum computing today is to perform nearly perfect gate operations. With trapped ions, initialization, readout, and single-qubit operations have already been demonstrated by various groups with very high fidelity. The implementation of a two-qubit gate operation is more involved as it demands coupling the internal states of two ions separated by a distance many orders of magnitude larger than the Bohr radius. Ideally, the gate should operate at high speed and with a fidelity allowing for fault-tolerant quantum computation. To comply with the latter requirement, the gate operation should not couple the qubits dissipatively to the environment (for example, by spontaneous emission), nor should the qubits be affected by dephasing mechanisms like fluctuating magnetic fields or path lengths in the optical setup. With trapped ions, impressive progress toward high-fidelity two-qubit gates has been made over the last couple of years, yet all current experimental realizations [1–4] achieve fidelities not exceeding 97% and thus still fall short of coming close to the desired level of precision [5].

Optical Raman fields are a convenient tool to create strong spin-dependent forces on hyperfine ion qubits [1,3,6,7], where "spin" refers to the effective Pauli spin associated with the qubit's two-level system. Acting on a single ion, these forces can entangle the internal-spin and motional degrees of freedom of the ion [6,7]; following disentanglement, the ion acquires a net geometric phase that is spin dependent [8]. When the force is exerted simultaneously on two ions, the geometric phase depends nonlinearly on their spins and can be used to entangle the ions' internal degrees of freedom [1,3,8–10]. Quantum gates based on these collective laser-ion interactions come in two flavors. In the first approach, experimentally pursued by Leibfried *et al.* [1], a moving standing wave pattern of two laser beams induces, for properly chosen laser beam polarizations, a spatially varying state-dependent ac Stark shift. This generates in turn a σ^z-dependent force, i.e., a force on the ions whose amplitude depends on the internal energy states. The resulting controlled-phase gate, called a $\hat{\sigma}^z$ gate, is remarkably fast and robust.

As the Raman coupling in [1] is mediated by a short-lived $P_{1/2}$ level [see Fig. 1(a)], spontaneous emission dominates the error budget even for a large detuning Δ from the virtual level [11]. Unfortunately, the use of a large Raman detunning makes the gate operation very inefficient when acting on "clock" states (states whose energy splitting is first-order independent of changes of the magnetic field) [7,12,13], for no differential Stark shift can be induced on them in the limit $\Delta \gg \omega_0$ [13], where ω_0 is the hyperfine structure splitting of the qubit states. Therefore, the remarkably long coherence times [14] available for clock states cannot directly be combined with the intrinsic robustness of the $\hat{\sigma}^z$ gate when based on Raman transitions with electric dipole coupling.

The second type of collective quantum gate, pioneered by Sørensen and Mølmer [9], entangles the qubits by inducing collective spin flips of both ions. It is based on a $\hat{\sigma}^\phi$-dependent force, with $\hat{\sigma}^\phi$ being a linear combination of

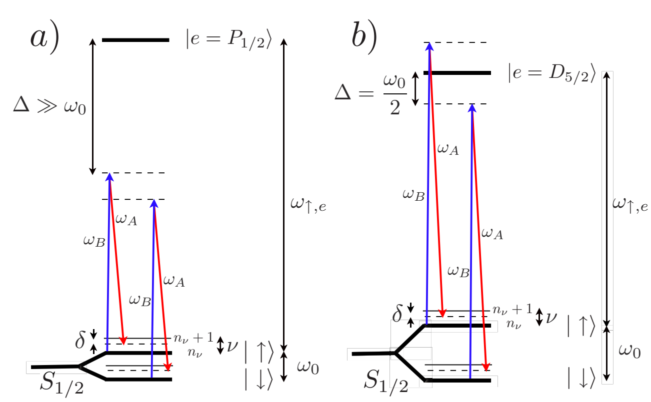

FIG. 1. (Color online) The usual implementation (a) uses a $P_{1/2}$ level as the excited state and works with $\Delta \gg \omega_0$; the qubit states are magnetic-field-sensitive and the differential coupling is achieved mainly through polarization discrimination. In the implementation (b) the excited state is a $D_{5/2}$ metastable level and Δ is small enough for the qubit states to be spectrally discriminated, which allows for the use of clock states. Maximal discrimination occurs at $\Delta=\omega_0/2$, where the effective coupling of $|\uparrow\rangle$ to its motional sideband is exactly opposite to that of $|\downarrow\rangle$.

the Pauli spin operators $\hat{\sigma}^x$ and $\hat{\sigma}^y$, capable of operating on clock states [7]. Even though this gate is formally equivalent to the $\hat{\sigma}^z$ gate in a rotated basis, it has the disadvantage that it involves spin flips, which make the gate more sensitive to magnetic field fluctuations than the $\hat{\sigma}^z$ gate [1]. Spin flips also constitute a drawback for quantum computation in decoherence-free subspaces protected against collective dephasing, for which controlled-phase gates are naturally better suited [15]. Furthermore, the required laser beam configuration gives rise to strong sensitivity of the qubits' coherences to the optical phases of the driving fields, constituting a serious limiting factor to the fidelity of the gate [16] unless special spin echo techniques are applied within the gate operation [7,13]. In addition, for this type of gate, spontaneous emission also sets a fundamental major limit to the fidelity.

In this paper, we investigate how to overcome the $\hat{\sigma}^z$ gate's spontaneous emission problem and its inefficiency with clock states by using electric quadrupole transitions for mediating the Raman coupling. The main idea is to induce a state-dependent force on the ions via Raman lasers tuned close to a narrow transition. We illustrate the idea with the $S_{1/2}\leftrightarrow D_{5/2}$ transition in $^{43}\mathrm{Ca}^+$, but it can also be applied to other ion species with a similar level structure [17]. Two noncopropagating lasers are tuned such that the two qubit levels, $|\uparrow\rangle\equiv|S_{1/2}(F=3,m_F=0)\rangle$ and $|\downarrow\rangle\equiv|S_{1/2}(F=4,m_F=0)\rangle$, experience opposite detunings from the metastable $D_{5/2}$ level [see Fig. 1(b)]. Two ions placed inside the standing wave pattern created by such laser beams experience a force. The direction and amplitude of the force on each ion depend jointly on the ions' internal state configuration, the distance between them, and the collective motional mode chosen. As in Ref. [1], a conditional dynamics is achieved by introducing a frequency difference of both beams close to the frequency of a vibrational mode of the ion string. As a result, the state-dependent force becomes periodic and excites, for instance, the center-of-mass (c.m.) mode if and only if the two ions are in opposite internal states and separated by a semi-integer multiple of wavelengths. The periodicity induced by the detuning from the vibrational frequency ensures that the ion string eventually returns to its initial motional state. During this process, however, the ion string picks up a phase proportional to its excitation, which allows one to realize a maximally entangling controlled-phase gate.

Distinguishing between the internal ionic levels only via their respective detunings works for any pair of qubit levels with a sufficiently large energy difference, regardless of their magnetic properties, in particular for clock states. However, it requires that the mediator level (the $D_{5/2}$ level in our example) is long lived, to achieve a reasonably small spontaneous emission rate. Concentrating again on $^{43}\mathrm{Ca}^+$, the $D_{5/2}$ level has a lifetime of about 1 s, such that the probability of spontaneous emission of a photon from both ions, and for a Raman detuning of half the energy splitting of the ground-state hyperfine structure, is well below the asymptotic threshold for fault-tolerant quantum computation found in [5].

We now describe the emergence of the state-dependent force via spectral discrimination and the implementation of the $\hat{\sigma}^z$ gate. For a more detailed explanation of general spin-dependent forces we refer the reader to Ref. [13] and references therein. We are interested in the implementation of the interaction Hamiltonian

$$\hat{H}_{\mathrm{int}_i}=\sum_{m_i}(F_{0_{m_i,i}}z_{\nu_{\mathrm{c.m.}}}\hat{a}^{\dagger}_{\mathrm{c.m.}}e^{i\delta t}+\mathrm{H.c.})|m_i\rangle\langle m_i|, \tag{1}$$

with $m_i=\uparrow$ or $\downarrow$ being the pseudospin state of ion i, for $i=1$ or 2. Hamiltonian (1) describes a particle with internal states $|m_i\rangle$ trapped in a harmonic potential of frequency $\nu_{\mathrm{c.m.}}$ and driven by a classical periodic force of amplitude $F_{0_{m_i,i}}$ and frequency $\delta\ll\nu_{\mathrm{c.m.}}$. We consider the collective center-of-mass motional mode as the harmonic oscillator because it exhibits lower levels of dephasing [18]. Nevertheless, the treatment can be straightforwardly applied to the stretch mode, too. In Eq. (1), $z_{\nu_{\mathrm{c.m.}}}\equiv\sqrt{\hbar/2M\nu_{\mathrm{c.m.}}}$, where M is the single-ion mass, $\nu_{\mathrm{c.m.}}$ is the root mean square spread of the motional ground state wave packet, and $\hat{a}^{\dagger}_{\mathrm{c.m.}}$ is the creation operator of one phonon of the c.m. mode. Upon evolution with Hamiltonian (1), the oscillator is periodically driven through a circular trajectory in phase space. For an evolution time $T=2n\pi\delta^{-1}$, with $n\in\mathbb{N}$, it ends up back in its initial position, but with each state $|m_i\rangle$ having acquired a geometrical phase $\Phi(T=2n\pi\delta^{-1})\equiv 2n\pi|z_{\nu_{\mathrm{c.m.}}}F_{0_{m_i,i}}/\delta\hbar|^2$. When the force is exerted simultaneously on both ions, the phase eventually acquired by each composite state $|m_1,m_2\rangle$ can be set to yield the maximally entangling $\hat{\sigma}^z$ gate by properly controlling the values of $F_{0_{m_1,1}}$, $F_{0_{m_2,2}}$, and δ, as is described below.

Figure 1(b) sketches the relevant frequencies, $\omega_A\equiv\omega_{\uparrow,e}+\Delta-(\nu_{\mathrm{c.m.}}-\delta)$ and $\omega_B\equiv\omega_{\uparrow,e}+\Delta$, $\omega_B-\omega_A=\nu_{\mathrm{c.m.}}-\delta$, with $\omega_{\uparrow,e}$ being the frequency difference between the excited state $|e\rangle$ and $|\uparrow\rangle$, and ω_0 between $|\uparrow\rangle$ and $|\downarrow\rangle$. We have $\Delta\gg\nu_{\mathrm{c.m.}}\gg\delta$, while Δ and ω_0 are of the same order of magnitude. Since the laser detuning Δ is still much larger than the $D_{5/2}$ state's hyperfine structure, we can treat the latter as an effective single level without internal structure. The individual interaction Hamiltonian in the Schrödinger picture and optical rotating-wave approximation (RWA) are then given by $\hat{H}'_i=\hbar\Sigma_{l,m_i}g_{l,i,m_i}|e\rangle\langle m_i|e^{i[k_{l_z}(z_{\nu_{\mathrm{c.m.}}}/\sqrt{2})(\hat{a}^{\dagger}_{\mathrm{c.m.}}+\hat{a}_{\mathrm{c.m.}})-\omega_l t-\varphi_l+k_{l_z}z_{0_i}]}+\mathrm{H.c.}$ [19]. The Rabi frequency g_{l,i,m_i}, of laser $l=A$ or B couples level $|m_i\rangle$ with $|e\rangle$ of ion i, k_{l_z} is the component of the lth laser's wave vector along the trap axis z, φ_l its optical phase, and z_{0_i} the equilibrium position of ion i. If (I) $|g_{l,i,\uparrow}|\ll\Delta$ and $|g_{l,i,\downarrow}|\ll|\Delta-\omega_0|$, and since $\Delta\approx|\Delta-\omega_0|$ is much larger than the excited state's linewidth, level $|e\rangle$ can be adiabatically eliminated. The latter, together with the RWA eliminating terms rotating at frequencies Δ and $\Delta-\omega_0$, yields the following effective Hamiltonians in the interaction picture: $\hat{H}'_i=\hbar\Sigma_{m_i}[\chi_{m_i,i}+(\theta_{m_i,i}e^{i[\eta_{\mathrm{c.m.}}(\hat{a}^{\dagger}_{\mathrm{c.m.}}e^{i\nu_{\mathrm{c.m.}}t}+\hat{a}_{\mathrm{c.m.}}e^{-i\nu_{\mathrm{c.m.}}t})-(\nu_{\mathrm{c.m.}}-\delta)t-\phi_i]}+\mathrm{H.c.})]|m_i\rangle\langle m_i|$. Here $\eta_{\mathrm{c.m.}}\equiv\Delta k_z z_{\nu_{\mathrm{c.m.}}}/\sqrt{2}$, with $\Delta k_z\equiv k_{B_z}-k_{A_z}$, is the Lamb-Dicke parameter and $\phi_i\equiv\varphi_B-\varphi_A-\Delta k_z z_{0_i}$. $\chi_{\uparrow,i}\equiv-(|g_{A,i,\uparrow}|^2+|g_{B,i,\uparrow}|^2)/\Delta$ and $\chi_{\downarrow,i}\equiv-(|g_{A,i,\downarrow}|^2+|g_{B,i,\downarrow}|^2)/(\Delta-\omega_0)$ are the time-averaged components of the ac Stark shift, and $\theta_{\uparrow,i}\equiv-g_{B,i,\uparrow}g^*_{A,i,\uparrow}/\Delta$ and $\theta_{\downarrow,i}\equiv-g_{B,i,\downarrow}g^*_{A,i,\downarrow}/(\Delta-\omega_0)$ its time-dependent components.

The last Hamiltonian still contains fast oscillations at frequency $\nu_{\text{c.m.}}$. In (II) the resolved sideband limit $|\theta_{m_i,i}| \ll \nu_{\text{c.m.}}$ only the stationary (nonoscillating) terms give a significant contribution to the effective Hamiltonian, whereas the others can be neglected under the RWA. Furthermore, (III) in the Lamb-Dicke limit $\eta^2_{\text{c.m.}}(n_{\text{c.m.}}+1/2)\ll 1$, where $n_{\text{c.m.}}$ is the mean population of the c.m. mode, only the terms linear in $\eta_{\text{c.m.}}$ contribute. Then the effective Hamiltonians are finally given by

$$\hat{H}_{\text{int}_i} = \hbar \sum_{m_i} [\chi_{m_i,i} + (i\theta_{m_i,i}\eta_{\text{c.m.}}e^{-i\phi_i}\hat{a}^\dagger_{\text{c.m.}}e^{i\delta t} + \text{H.c.})]|m_i\rangle\langle m_i|. \tag{2}$$

Let us momentarily disregard the time-averaged Stark shift from Hamiltonian (2) and consider only its time-dependent component that contains the vibrational operators generating the interaction between both qubits. Under this assumption it suffices to define $F_{0_{m_i,i}}z_{\nu_{\text{c.m.}}} \equiv i\hbar\theta_{m_i,i}\eta_{\text{c.m.}}e^{-i\phi_i}$ to identify Hamiltonian (2) with (1), realizing thus the desired $\hat{\sigma}^z$-dependent force on both ions. For simplicity, we take $g_{l,1,m}=g_{l,2,m}\equiv g_{l,m} \Rightarrow \theta_{m,1}=\theta_{m,2}\equiv\theta_m \Rightarrow |F_{0_{m,1}}|=|F_{0_{m,2}}|\equiv|F_{0_m}|$, as no individual laser addressing has been assumed. The extension to nonequal coupling though is straightforward. The phase difference between the forces applied to both ions is then determined by the ion spacing at equilibrium: $\phi_1-\phi_2 = \Delta k_z \Delta z_0$, with $\Delta z_0 \equiv z_{0_1}-z_{0_2}$. Here it is convenient to set the spacing equal to a semiinteger multiple of the optical wavelength: $\Delta k_z\Delta z_0=(2n+1)\pi$, so that both ions experience opposite forces. In this way the total force on the c.m. mode $F_{0_{m_1,m_2}}z_{\nu_{\text{c.m.}}} \equiv (F_{0_{m_1}}+F_{0_{m_2}})z_{\nu_{\text{c.m.}}} = \hbar i(\theta_{m_1}-\theta_{m_2})\eta_{\text{c.m.}}e^{-i\phi_1}$ is nonvanishing only for antialigned spins.

After one phase-space round trip of duration $T=2\pi\delta^{-1}$ (the shortest gate time possible) the composite states evolve as $|m_1,m_2\rangle \to |m_1,m_2\rangle$, for $m_1=m_2$; and $|m_1,m_2\rangle \to e^{i\Phi}|m_1,m_2\rangle$, for $m_1\neq m_2$, with $\Phi=2\pi|(\theta_\uparrow-\theta_\downarrow)\eta_{\text{c.m.}}\delta^{-1}|^2$. Maximal entanglement is achieved for $\Phi=\pi/2$; and the bigger the difference between $\theta_\uparrow$ and $\theta_\downarrow$, the faster the gate. Imposing thus $\Phi=\pi/2$ and using the definition of θ_m, the general discrimination condition for maximal entanglement is obtained:

$$\left|\frac{g_{B,\uparrow}g^*_{A,\uparrow}}{\Delta} - \frac{g_{B,\downarrow}g^*_{A,\downarrow}}{\Delta-\omega_0}\right| = \left|\frac{\delta}{2\eta_{\text{c.m.}}}\right|. \tag{3}$$

Since we are most interested in working with qubit states with the same magnetic properties no discrimination via polarization can take place, i.e., $g_{l,\uparrow}=g_{l,\downarrow}\equiv g_l$, for $l=A$ or B. Therefore, the only way to satisfy condition (3), which then reads $|g_Bg^*_A[\Delta^{-1}-(\Delta-\omega_0)^{-1}]|=|\delta/2\eta_{\text{c.m.}}|$, is through spectral discrimination. Maximal discrimination occurs at $\Delta=\omega_0/2$, when $\theta_\uparrow=-\theta_\downarrow$. As shown in Fig. 1(b), for this detuning, $|\uparrow\rangle$ couples to the excited state $|e\rangle$ through blue-detuned light and $|\downarrow\rangle$ through red-detuned light of the same intensity. So both states' effective couplings with the motional sideband (and therefore also the forces each spin state experiences) are exactly opposite. Thus the optimal form of condition (3) is

$$|g_Bg^*_A| = \left|\frac{\delta\omega_0}{8\eta_{\text{c.m.}}}\right|. \tag{4}$$

For $^{43}Ca^+$, the ground-state hyperfine splitting is $\omega_0=2\pi \times 3.226$ GHz. The resulting Raman detuning is 20 times larger than the hyperfine splitting of the $D_{5/2}$ manifold, so that the single-level approximation is comfortably satisfied. It is also much larger than the linewidth $\gamma_D=2\pi\times 0.18$ Hz. For the typical experimental parameters $\nu_{\text{c.m.}}=2\pi \times 1.2$ MHz, $\eta_{\text{c.m.}}=0.1$, and $\delta=2\pi\times 1$ kHz, and taking $|g_A| = |g_B|\equiv|g|$, the value $g=2\pi\times 2$ MHz is obtained from Eq. (4) for the optical quadrupole couplings. All the other approximations made in the derivation of Hamiltonian (2) are in turn well satisfied. They are (I) $|g|=2\pi\times 2\text{ MHz}\ll 2\pi \times 1.613\text{ GHz}=|\Delta-\omega_0|=\Delta$; (II) $|\theta_m|/\nu_{\text{c.m.}}=0.002\ll 1$; and (III) $\eta^2_{\text{c.m.}}(n_{\text{c.m.}}+1/2)=0.01(n_{\text{c.m.}}+1/2)$, which is much smaller than 1 for the mode populations of interest. On the other hand, the total duration of the gate (limited by the available amount of laser power) is $T=1$ ms, which is short as compared to the long coherence times expected for clock states [14]. To speed up the gate time to 100 μs, for example, a total laser power of about 1 W, when focusing the laser beams to waist sizes of 6 μm, would be required.

Not all types of spontaneous emission affect the gate's performance equally [20]. The dominant source of gate error comes from inelastic Raman scattering which affects the ion-qubit coherences directly, whereas elastic Rayleigh scattering can only affect the gate's fidelity indirectly through the ions' recoils. In what follows, we calculate the total probability of spontaneous photon scattering and simply take it as an overestimated figure of merit for the gate error. The mean probability of off-resonant direct excitation of the excited state $|D_{5/2}\rangle$ under the action of the two $(\omega_0/2)$-detuned lasers is approximately $p_{\text{off}}=8|g|^2/\omega_0^2\equiv 2\times 10^{-6}$. The total probability of spontaneous emission from both ions during the gate time $T=2\pi\delta^{-1}$ is then $p_{\text{T}}\equiv 2\times p_{\text{off}}\times\gamma_D\times 2\pi\delta^{-1}\equiv 2 \times 8|g|^2/\omega_0^2\times\gamma_D\times 2\pi\omega_0/8|g|^2\eta_{\text{c.m.}}\equiv(4\pi/\eta_{\text{c.m.}})\gamma_D/\omega_0\equiv 6.3 \times 10^{-9}$, where condition (4) has been used. This value is more than four orders of magnitude below the asymptotic threshold value set in [5] for fault-tolerant quantum computation. When it comes to choosing a specific ion as a quantum-information carrier in the case of gate operations mediated by a short-lived P level, it seems favorable to avoid ion species with low-lying D levels [20]. The gate scheme proposed here not only works for any ion species with a low-lying narrow transition, but also it is exactly the use of the low-lying narrow transition as the mediator that enables an error threshold four orders of magnitude smaller than for gates mediated by short-lived P levels.

Let us now go back to the time-averaged Stark shifts disregarded from Hamiltonian (2). In principle, the single-ion phases they induce can be compensated at the end of the evolution by single-ion gates. As for the robustness of an implementation, however, they are very important. Since $|\chi_{m_i}|$ is about 20 times as big as $|\theta_{m_i}\eta_{\text{c.m.}}|$, the acquired single-ion phases are much larger than the desired conditional $\pi/2$ phase, which makes the gate's performance extremely sensitive to laser-intensity fluctuations. One way to overcome this is to add additional frequencies onto the gate laser so as to compensate the time-averaged components of the Stark shift without compensating its time-varying components [21]. Alternatively, a spin-echo technique can be applied. In this approach, the gate is divided into two phase-space round trips, in each of which half the desired conditional phase is acquired, with a pulse interchanging the qubit populations in the middle. This increases the gate time by a factor of $\sqrt{2}$, but for laser power fluctuations slower than the gate time both ions pick up the same final single-ion phase. These two techniques can also be combined.

Since the scheme is based on the use of weak transitions, the large amount of laser power it requires to achieve short gate times is somewhat challenging. In a proof-of-principle experiment, this technical drawback can be circumvented using alternative qubit encodings that decrease the required laser power. For instance, one can map the qubit onto clock states of the hyperfine splitting of the $D_{5/2}$ manifold. Hereby the qubit transition frequency is reduced by almost a factor of 500, so that the required laser couplings are reduced by more than one order of magnitude. A ground-state sublevel serves as the Raman mediator, and coupling to the other Zeeman sublevels of the ground state manifold can be avoided by properly choosing the laser polarizations. Since the $D_{5/2}$ level is now occupied by both qubit states throughout the gate, the probability of spontaneous emission is directly given by $p_{\mathrm{T}} \equiv 2\times\gamma_D\times T$. For instance, for an estimated gate time of $T=100\ \mu$s ($g\approx 2\pi\times 285$ kHz) including mapping of the qubits, the spontaneous scattering per gate run would still be as low as $p_{\mathrm{T}}=2\times 10^{-4}$. Alternatively, another possible encoding is provided by one clock state from $S_{1/2}$ and another from $D_{5/2}$, where values of $g\approx 2\pi\times 210$ kHz and $p_{\mathrm{T}}\approx 10^{-4}$ are expected [22].

We propose an implementation of the $\hat{\sigma}^z$ gate on hyperfine ground-state qubits that overcomes the two main problems of previous implementations: spontaneous emission and inefficiency with clock states. The gate is driven by forces exerted by two beams in a Raman configuration tuned close to a narrow transition, and state dependency is achieved by a small frequency detuning instead of polarizations. We discuss the idea for $^{43}Ca^+$, but it can also be applied to other ion species with a similar level structure. We find a total probability of spontaneous emission per gate run of less than 10^{-8}, thus eliminating the main source of gate infidelity of previous implementations with magnetic-field-sensitive states. In order to achieve short gate times, the scheme requires a large amount of laser power. We show two examples of ways to circumvent this by using alternative qubit encodings. With increasingly powerful laser sources though, our $\hat{\sigma}^z$ gate can set a standard for robust high-fidelity entanglement creation in the future large-scale ion-trap quantum computer, where the qubit encoding will be that of hyperfine ground-state sublevels. With this scheme it seems possible to reach the fault-tolerant threshold.

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