

Nonparaxial effects on laser-qubit operations

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Tightly focused laser beams, or optical tweezers, are essential for analog and digital quantum simulation with neutral atoms and trapped ions. Despite this, most of the current intuition and theoretical treatment utilizes the paraxial approximation, which is an insufficient description at the focus of tightly focused optical tweezers. We develop an analytic model, which we use in tandem with numerical simulations, to quantify how nonparaxial effects will manifest in the next generation of scalable quantum hardware, where tightly focused beams are used for individual qubit control. In particular, we calculate the light potentials of Gaussian and Laguerre-Gaussian beams driving the quadrupole $^2S_{1/2} \rightarrow ^2D_{5/2}$ transition in $^{40}\text{Ca}^+$. Longitudinal field components in the beam center cause spatially dependent Rabi frequencies and ac Stark shifts, leading to unexpected qubit-motion coupling. We characterize single- and two-qubit gate infidelities due to this effect with an analytic model and numerical simulation. We identify regimes where nonparaxial effects should be taken into account for high-precision quantum control, and highlight that the effects are potentially more severe for the case of neutral atom and molecule addressing.

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I. INTRODUCTION

Optical tweezers have enabled remarkable progress in cold atomic physics in the last decade. On one hand, optical tweezers can hold hundreds of neutral atoms to form large arrays of atomic qubits, paving the way for the construction of a scalable quantum computer [1–8]. On the other hand, in trapped-ion platforms for quantum simulation and computation, tightly focused laser beams are used to address individual ions and prepare, manipulate, and measure their internal (qubit) state [9–12]. Furthermore, optical tweezers may be used to modify the local confinement of trapped ions [13–19] with applications in quantum computing and simulation. As the ions are typically separated by several micrometers [20], it is crucial to obtain the smallest possible foci for the addressing lasers to avoid crosstalk.

In the above applications, the tweezer light fields are typically considered to be Gaussian and described within the paraxial approximation. In this approximation, the divergence angle of the light field with respect to the optical axis is considered to be small. However, close to the focus, large

deviations from the paraxial approximation appear [21–25]. These may cause strong gradients in the polarization components along the tweezer propagation direction, which in turn leads to the appearance of state-dependent forces in the direction perpendicular to the tweezer [22,26–28].

In trapped ions, these effects may lead to a loss of qubit coherence caused by qubit-motion entanglement [29–31]. The effect is potentially harmful as the forces typically point along the weakly confined axial direction of the ion crystal, which is harder to cool due to its broad spectral range [20]. In this paper, we present a detailed study of adverse nonparaxial effects for the case of an optical qubit encoded in a $^{40}\text{Ca}^+$ ion that is addressed by a tightly focused laser connecting the qubit states in the Zeeman manifold of $^2S_{1/2}$ and $^2D_{5/2}$. We calculate the coupling of the tweezer on both the $^2S_{1/2} \rightarrow ^2D_{5/2}$ quadrupole transition and the strongest dipole transitions in $^{40}\text{Ca}^+$. This enables us to determine spatially dependent Stark shifts on the qubit states [32]. We calculate the fidelity loss for single- and two-qubit gates due to the tweezer-induced qubit-motion and qubit-qubit coupling. While the resulting errors remain below typical fault-tolerant thresholds [33], we identify regimes where they become more significant and provide strategies to suppress them. This accounts for an overlooked practical challenge for the next generation of quantum computers, which seeks high-precision control of atomic qubits. Our calculations may be straightforwardly extended to ions with similar level schemes such as Sr^+ and Ba^+ , and the techniques presented may also be applied to neutral atoms and molecules.

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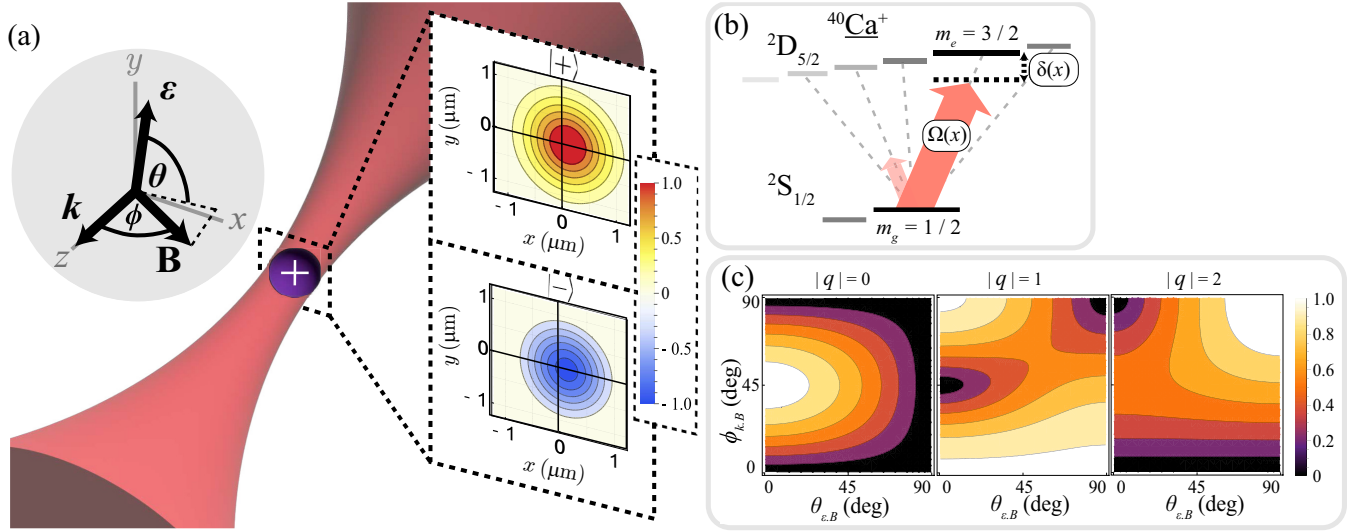


FIG. 1. Tweezer setup and orientation. (a) We consider a tightly focused beam resonantly driving a quadrupole transition in a trapped ion. In the gray circle, we illustrate the coordinate system, with angle ϕ describing the angle between the magnetic field $\mathbf{B}$ and propagation vector $\hat{k}$, and angle θ the orientation of the polarization $\hat{\epsilon}$ vector with respect to the projection of $\mathbf{B}$ on the transverse plane. For the case in which $\mathbf{B} \parallel \hat{\epsilon} \parallel y$ (as studied below), we show the transverse potentials E/h (in units MHz) of the dressed qubit states $\{|+\rangle, |-\rangle\}$, which are displaced in the x direction by approximately $\lambda/2\pi$. An off-axis field gradient and curvature at the ion's position can induce a qubit-motion coupling error. (b) Simplified level scheme of $^{40}\text{Ca}^+$ showing the resonant quadrupole transition, with a position-dependent Rabi frequency $\Omega(x)$ and ac Stark shift $\delta(x)$. (c) Geometric dependence of the quadrupole coupling ($m_g \rightarrow m_g + q$ for $q = 0, \pm 1, \pm 2$) at the beam center, as a function of angles θ and ϕ , which are defined in the text and shown in Fig. 1. Here, the beam waist is $w_0 = \lambda = 729$ nm. Light (dark) shadings signify high (low) coupling strength.

II. SETUP

We consider a trapped $^{40}\text{Ca}^+$ ion being addressed by a tightly focused beam, resonantly driving the quadrupole transition between qubit states $|0\rangle = 4^2S_{1/2}$ ($m_g = 1/2$) and $|1\rangle = 3^2D_{5/2}$ ($m_e = 3/2$), as shown in Fig. 1(b). In this section, we derive the following Hamiltonian:

$$H = H_{\text{AL}} + H_Z + H_\alpha. \quad (1)$$

Here, H_{AL} is the atom-light Hamiltonian describing dipole and quadrupole interactions. For this, we first consider a Gaussian beam beyond the paraxial approximation, with the electric field components and their derivatives driving dipole and quadrupole interactions, respectively. H_Z is the Zeeman Hamiltonian that describes the effect of an external magnetic field. The effect of off-resonant dipole coupling is included in term H_α . Finally, we use the two-level approximation to study the resulting qubit-motion entangling errors. Note that the following methods are applicable to other qubit platforms (e.g., neutral atoms) with similar level structures.

A. Electric field: beyond the paraxial approximation

In the paraxial approximation, the electric field of a Gaussian beam is taken to be uniformly polarized. Then, for a beam with transverse polarization propagating in the $\hat{z}$ direction, the electric field is given by

$$\begin{aligned} \mathbf{E}(\mathbf{r}, t) &= \text{Re}[f(\mathbf{r})\hat{\epsilon} e^{i(kz - \omega t)}] \\ &= \mathbf{E}^+ e^{i\omega t} + \mathbf{E}^- e^{-i\omega t}, \end{aligned} \quad (2)$$

where $\hat{\epsilon} \cdot \hat{z} = 0$ and the mode function

$$\begin{aligned} f(\mathbf{r}) &= \frac{E_0}{1 + iz/z_0} \exp\left(-\frac{k}{2} \frac{\rho^2}{z_0 + iz}\right) \\ &= E_0 \frac{w_0}{w(z)} \exp\left(-\frac{\rho^2}{w^2(z)} + ik \frac{\rho^2}{2R(z)} + i\psi(z)\right). \end{aligned}$$

Here, $\rho = \sqrt{x^2 + y^2}$, $z_0 = \pi w_0^2/\lambda = kw_0^2/2$ is the Rayleigh range, $w(z) = w_0\sqrt{1 + (z/z_0)^2}$ is the Gaussian waist, w_0 is the minimum waist, $R(z) = (z^2 + z_0^2)/z$ is the wave front radius of curvature, and $\psi(z) = -\arctan(z/z_0)$ is the Gouy phase.

In this paper, we consider nonparaxial effects that occur in tightly focused beams, e.g., near the focal plane of optical tweezers, where we can no longer assume that the polarization is uniform. Note that Eq. (2) is not strictly a solution of the Helmholtz wave equation. In fact, in the tight-focusing regime, longitudinal field components appear and the polarization becomes strongly position dependent.

A simple way to obtain a first-order correction to the paraxial approximation [34–36] is to start from the vector potential $\mathbf{A}(\mathbf{r}, t)$ with the same form as Eq. (2). If the Lorenz condition $\nabla \cdot \mathbf{A} + (1/c^2)\partial\Phi/\partial t = 0$ is satisfied, the corresponding $\mathbf{E}(\mathbf{r}, t)$ can be expressed entirely in terms of $\mathbf{A}(\mathbf{r}, t)$. Neglecting the spatial derivatives of higher than first order, the electric field in the focal plane $z = 0$ is given by [37,38]

$$\mathbf{E}(\rho, t) \approx \text{Re}\left[\left(\hat{\epsilon} - \frac{i(\epsilon_x x + \epsilon_y y)}{z_0} \hat{z}\right) f(\mathbf{r}) e^{i(kz - \omega t)}\right]. \quad (3)$$

Equation (3) is the lowest-order correction beyond the paraxial approximation and contains a longitudinal field component that is $\pi/2$ out of phase with the transverse component

and vanishes on the optical axis. While Eq. (3) is not a solution to the Helmholtz wave equation, it is a good approximation for the regime considered in this paper. However, in an extremely tightly focused regime, the solution will no longer be valid and one should instead use exact electric field patterns, which can be obtained numerically. This can be done using the angular spectrum representation, essentially writing $\mathbf{E}(\mathbf{r}, t)$ as a superposition of plane waves [22,37].

B. Atom-light Hamiltonian

The atom-light Hamiltonian driving dipole (E1) and quadrupole (E2) transitions is given by

$$H_{\text{AL}}(\hat{\mathbf{r}}) = H_{E1} + H_{E2} \\ = \hat{\mathbf{r}}_i E_i + \hat{\mathbf{r}}_i \hat{\mathbf{r}}_j \partial_i E_j, \quad (4)$$

where we have used Einstein's summation convention and set the electron's charge to 1. Here, $\hat{\mathbf{r}}$ is the position operator of the electron relative to the center of mass of the atom and E_i is the electric field component of the light along the i axis evaluated at the center of mass. We use Eq. (3) to evaluate the electric field components.

It is convenient to express $\hat{\mathbf{r}}$ in spherical components, because its matrix elements are then easily evaluated as Clebsch-Gordan coefficients. Using the definitions

$$\hat{r}_{\pm 1} = \mp \frac{1}{\sqrt{2}}(\hat{x} \pm i\hat{y}), \quad \hat{r}_0 = \hat{z}, \quad (5)$$

the dipole coupling Hamiltonian can be written as

$$H_{E1} = \sum_q (-1)^q \hat{r}_q E_{-q} \\ = -\hat{r}_1 E_{-1} + \hat{r}_0 E_0 - \hat{r}_{-1} E_1 \\ = \hat{r}_1 \frac{-E_x + iE_y}{\sqrt{2}} + \hat{r}_0 E_z + \hat{r}_{-1} \frac{E_x + iE_y}{\sqrt{2}},$$

where $\langle J_e, m_e | \hat{r}_q | J_g, m_g \rangle \propto C_{J_g, m_g, 1, q}^{J_e, m_e = m_g + q}$ and

$$E_{\pm 1} = \mp \frac{1}{\sqrt{2}}(E_x \pm iE_y), \quad E_0 = E_z. \quad (6)$$

Next, we evaluate the quadrupole coupling Hamiltonian. The quadrupole coupling is the product of the dyadic $r_i r_j \equiv Q_{ij}$ and the field gradient tensor $\partial_i E_j = (\nabla \mathbf{E})_{ij}$. Both may be decomposed into their irreducible spherical tensor components, $\nabla \mathbf{E} = (\nabla \mathbf{E})^{(0)} + (\nabla \mathbf{E})^{(1)} + (\nabla \mathbf{E})^{(2)}$, of rank 0, 1, and 2, respectively. A similar decomposition can be performed for the dyadic Q . We note that by symmetry $Q^{(1)} = 0$ and $(\nabla \mathbf{E})_0^{(0)} = -(1/\sqrt{3})\partial_z E_i = 0$ as required by the Maxwell's equations. Thus, in the E2 coupling only the rank-2 components remain and we find [20,39],

$$H_{E2} = \sum_q (-1)^q Q_q^{(2)} (\nabla \mathbf{E})_{-q}^{(2)}. \quad (7)$$

The gradient is expressed in Cartesian components as [40]

$$(\nabla \mathbf{E})_{\pm 2}^{(2)} = \frac{1}{2}(\partial_x \pm i\partial_y)(E_x \pm iE_y), \quad (8)$$

$$(\nabla \mathbf{E})_{\pm 1}^{(2)} = \frac{1}{2}[\mp \partial_z(E_x \pm iE_y) \mp (\partial_x \pm i\partial_y)E_z], \quad (9)$$

$$(\nabla \mathbf{E})_0^{(2)} = \frac{\sqrt{6}}{2}\partial_z E_z, \quad (10)$$

where we have used $\partial_i E_i = 0$ to simplify the equation for $(\nabla \mathbf{E})_0^{(2)}$. Finally, in the irreducible spherical tensor components representation, Eq. (7) can be written as

$$H_{E2} = \frac{1}{2}\{Q_2^{(2)}(\partial_x - i\partial_y)(E_x - iE_y) \\ + Q_1^{(2)}[-\partial_z(E_x - iE_y) - (\partial_x - i\partial_y)E_z] \\ + Q_0^{(2)}\sqrt{6}\partial_z E_z + \\ + Q_{-1}^{(2)}[\partial_z(E_x + iE_y) + (\partial_x + i\partial_y)E_z] \\ + Q_{-2}^{(2)}(\partial_x + i\partial_y)(E_x + iE_y)\}, \quad (11)$$

where $\langle J_e, m_e | Q_q^{(2)} | J_g, m_g \rangle \propto C_{J_g, m_g, 2, q}^{J_e, m_e = m_g + q}$.

C. Zeeman Hamiltonian

The energy levels of the atom shift in the presence of an external magnetic field, as given by the Zeeman Hamiltonian

$$H_Z = g_j \mu_B \mathbf{B} \cdot \hat{\mathbf{J}}. \quad (12)$$

Here, g_j is the Lande g factor, μ_B is the Bohr magneton, $\mathbf{B}$ is the magnetic field, and $\hat{\mathbf{J}}$ is a vector of angular-momentum operators for a particular angular momentum manifold. For instance, for $J_g = 1/2$ these are the Pauli matrices $\hat{J}_i = \hat{\sigma}_i/2$. We diagonalize H_Z to define the quantization axis along the magnetic field. The transformed H_{AL} in the new basis specified by the eigenvectors of H_Z is denoted by $\tilde{H}_{\text{AL}}$.

D. Geometric dependence

To make the m_j states in $|0\rangle$ and $|1\rangle$ resonant, we must make a suitable choice of magnetic field $\mathbf{B}$ orientation, polarization $\hat{\mathbf{e}}$, and laser frequency. From Eq. (7), the quadrupole Rabi frequency (in angular frequency units) between two m_j states is

$$\Omega_{E2, m_g, m_e} = \frac{ea_0^2}{\hbar} Q_{\text{red}} C_{J_g, m_g, 2, q}^{J_e, m_e} (-1)^q (\tilde{\nabla} \mathbf{E})_{-q}^{(2)}, \quad (13)$$

with $Q_{\text{red}} = \frac{\langle J_e || Q^{(2)} || J_g \rangle}{\sqrt{2J_e + 1}}$ the reduced quadrupole moment in atomic units [41], e the elementary charge, and a_0 the Bohr radius. We use $\tilde{\nabla}$ to denote the gradient in the coordinates specified by the quantization axis set by $\mathbf{B}$. The field gradients $(\tilde{\nabla} \mathbf{E})_{-q}^{(2)}$ define the spatial profile of the Rabi frequency. In Fig. 1(c), we find the relative amplitude of $(\tilde{\nabla} \mathbf{E})_{-q}^{(2)}$ (normalized between 0 and 1) at the beam center, as a function of the angle between the magnetic field direction and propagation vector $\vec{k}$ (ϕ) and the angle between the linear polarization $\hat{\mathbf{e}}$ and the magnetic field projection on the transverse plane (θ) [42]. We find that the *relative* coupling strength does not change in the presence of nonparaxial effects and has no dependence on the beam waist. However, we do note a small change in the amplitude due to nonparaxial effects at the beam center, as discussed in Sec. III.

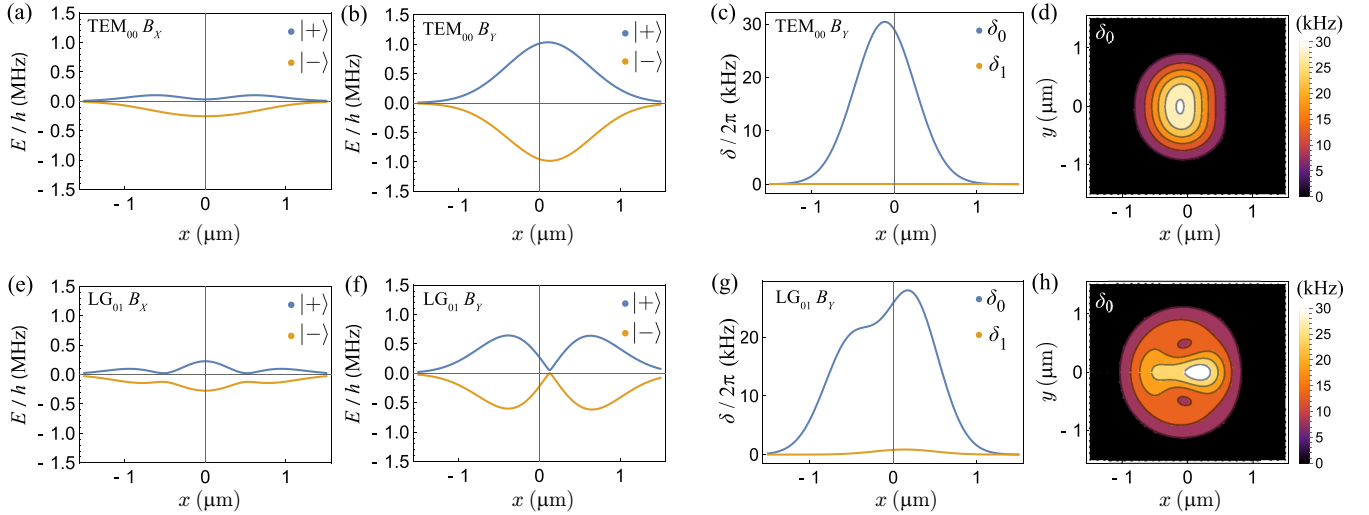


FIG. 2. Potential and light shifts. Potential of the dressed qubit states $\{|+\rangle, |-\rangle\}$ at the focus of an optical tweezer resonantly driving the quadrupole $^2S_{1/2} \rightarrow ^2D_{5/2}$ transition in $^{40}\text{Ca}^+$. (a), (b) Potential for a Gaussian beam TEM_{00} as a function of x (with $y = 0$ and $z = 0$), with linear polarization in the y direction, and magnetic fields in the x and y directions. The laser parameters are $P_0 = 10 \mu\text{W}$ and $w_0 = 729 \text{ nm}$. (c) AC Stark shifts of the qubit states as a function of x , with magnetic field B_y . (d) The dominant Stark shift as a transverse (x - y) contour plot in the focal plane ($z = 0$). Light (dark) regions signify a large (small) Stark shift. (e)–(h) As above for a Laguerre-Gaussian beam LG_{01} .

E. Off-resonant dipole coupling

To include the effect of off-resonant dipole coupling, we extract the reduced dipole moments for all relevant dipole transitions from Ref. [43], and from these calculate the scalar, vector, and tensor polarizabilities (α_s , α_v , and α_t , respectively) of each m_j state. The resulting Hamiltonian term H_α , which is solely due to off-resonant dipole coupling, is given by

$$H_\alpha = -\alpha_s E_0^2 - \frac{\alpha_v}{J} i(\mathbf{E}^- \times \mathbf{E}^+) \cdot \hat{\mathbf{J}} - \frac{3\alpha_t}{J(2J-1)} \left(\frac{1}{2} \{\mathbf{E}^+ \cdot \hat{\mathbf{J}}, \mathbf{E}^- \cdot \hat{\mathbf{J}}\} - \frac{1}{3} J(J+1) E_0^2 \right),$$

where $\{\cdot, \cdot\}$ is the anticommutator and $\hat{\mathbf{J}}$ are the angular momentum operators defined previously [44]. We arrive at the full Hamiltonian

$$H_1 = \tilde{H}_{\text{AL}} + H_Z + \tilde{H}_\alpha, \quad (14)$$

where the tilde indicates that H_{AL} and H_α have been transformed to the quantization axis.

F. Two-level approximation

We use second-order perturbation theory to go from H_1 to H_2 , which acts on the qubit basis $\{|0\rangle, |1\rangle\}$,

$$H_2 = \hbar \begin{pmatrix} \Delta/2 + \delta_0 & \Omega \\ \Omega^* & -\Delta/2 + \delta_1 \end{pmatrix}. \quad (15)$$

Here, the diagonal energy shifts are the ac Stark shifts on the qubit states due to the dipole and quadrupole coupling to other m_j states, given by $\delta_i = \sum_k \Omega_{ik} \Omega_{ki} / \Delta_{ik}$, where $\Delta_{ik} = E_i - E_k$ is the energy difference between the qubit states $i = 0, 1$ and other m_j states $k = 2, \dots, 7$. Furthermore, off-resonant Raman coupling slightly shifts the Rabi frequency between the qubit states by $\Omega_s = \sum_k \Omega_{0k} \Omega_{k1} / \Delta_{kl}$, where l labels the

qubit state in the same manifold as state k . We include this effect in Eq. (15) via the definition of the Rabi frequency between the qubit states $\Omega = \Omega_{01} + \Omega_s$. We note that the two-level approximation to H_1 remains valid for the range of laser parameters considered here.

III. SIMULATED LIGHT POTENTIAL

The eigenvalues of H_2 give the light potentials in the dressed basis $\{|+\rangle, |-\rangle\}$, where $|+\rangle = c_1|0\rangle + c_2|1\rangle$ and $|-\rangle = c_1|1\rangle - c_2|0\rangle$ are a linear combination of the qubit states. In Figs. 2(a) and 2(b), we show the spatial variation of the eigenvalues with x , with y and z fixed at the beam center. The ion experiences a $|\mathbf{B}| = 5 \text{ G}$ field with (a) $\mathbf{B} = B_x$ perpendicular to the polarization along y ($\theta = 90^\circ$ and $\phi = 90^\circ$) and (b) $\mathbf{B} = B_y$ parallel to the polarization ($\theta = 0^\circ$ and $\phi = 90^\circ$). The qubit states are resonant at a detuning of $\Delta = 2\pi 5.6 \text{ MHz}$, and the Rabi frequency amplitude is $\Omega = 2\pi 1 \text{ MHz}$ for tweezer power $P_0 = 10 \mu\text{W}$ and waist $w_0 = \lambda = 729 \text{ nm}$.

Since the potential is primarily due to the Rabi frequency between the qubit states, it follows the same spatial profile. For B_x , the potential is suppressed and spatially symmetric about the origin. For B_y , we note that while the profile is Gaussian, it is shifted from the atom's center-of-mass position due to the optical Magnus effect, as we describe below. Moreover, we plot the potentials for a Laguerre-Gauss mode $\text{LG}_{p,l} = \text{LG}_{01}$ in Figs. 2(e)–2(h), and observe a similar shifted potential in the B_y case. We note that for the set of parameters considered here, the Rabi frequency shifts Ω_s due to off-resonant Raman coupling are negligible and on the order of 100 Hz. The light shifts due to off-resonant dipole coupling are also small, on the order of 1 kHz, and their effect on the potential profile can also be neglected.

We explore the dependence of the optical Magnus effect displacement on the beam waist. To this end, we determine

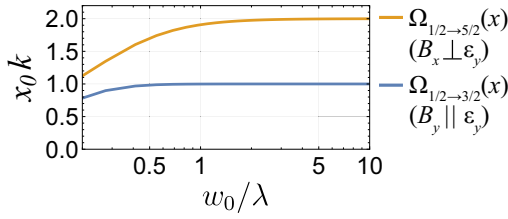


FIG. 3. Rabi frequency displacement. Displacement x_0 of the peak of the Rabi frequency $\Omega(x)$ as a function of waist size w_0 . The scale is logarithmic on the horizontal axis. When $\mathbf{B} \parallel \epsilon_y$, the resonant coupling $\Omega_{1/2 \rightarrow 3/2}(x)$ is displaced by $x_0 = k^{-1} = \lambda/2\pi$ (blue line) in the limit $w_0 \gg \lambda$. When $\mathbf{B} \perp \epsilon_y$, the resonant coupling $\Omega_{1/2 \rightarrow 5/2}(x)$ is displaced by $x_0 = 2k^{-1} = \lambda/\pi$ (orange line) in the same limit. For very small beam waists $w_0 \ll \lambda$, the displacement in both cases decreases, although this is typically below the diffraction limit.

the position of the peak (x_0) of $\Omega(x)$ by solving $\frac{\partial \Omega}{\partial x}|_{x=x_0} = 0$ to characterize how x_0 shifts in the direction of the focal plane. We consider the case of (1) $\mathbf{B} = B_y \parallel \epsilon_y$ and (2) $\mathbf{B} = B_x \perp \epsilon_y$. In the first case, the coupling $\Omega_{E2,1/2,3/2}(x)$ is resonant and x_0 approaches $k^{-1} = \lambda/2\pi$ as $w_0 \gg \lambda$, as shown in Fig. 3. In the second case, the displacement of resonant coupling $\Omega_{E2,1/2,5/2}(x)$ approaches $2k^{-1} = \lambda/\pi$ as $w_0 \gg \lambda$ (see Fig. 3). In both cases, for very small beam waists $w_0 \ll \lambda$ (which are typically below the diffraction limit) x_0 decreases. Finally, we note that when q is negative, the peak is displaced to the left instead of to the right (i.e., for $\Omega_{E2,1/2,-1/2}$, x_0 approaches $-\lambda/2\pi$ as $w_0 \gg \lambda$). We highlight that the displacement remains present even in the paraxial limit ($w_0 \gg \lambda$); however, the effects due to the beam curvature and gradient subside in this regime.

For the case studied here, we trace the asymmetry of the optical Magnus effect displacement to Eq. (11), line 2; specifically the second term containing circular gradients of the longitudinal field (which are subsequently rotated to the quantization axis). This term causes the displacement $x = \pm k^{-1}$ depending on both the sign of $\mathbf{B}$ and the change in angular momentum projection $q = \pm 1$. For the case of a dipole transition, the intuitive picture of the optical Magnus effect is due to the interplay of the spin-orbit coupling within the beam: As the beam is focused, the opposite curvature of the Poynting vector on either side causes the circularly polarized field components (σ^+ and σ^-) to shift off-axis. However, for the quadrupole transition considered here, the sign of the circular gradients— $(\partial_x \pm i\partial_y)$ in Eq. (11)—causes the asymmetric displacement of the Rabi frequency.

The ac Stark shifts δ_i are also shown in Fig. 2. We only show the B_y case due to the Stark shifts being much smaller for B_x . We note that the spatial profile is different from the Rabi frequency and, in particular, the displacement is in the opposite direction. This is due to the dominant contribution to δ_i ($\Omega_{E2,1/2,-1/2}$) being centered at $x \approx -\lambda/2\pi$. The Stark shift scales with the square of the Rabi frequency amplitude, $\delta \propto |\Omega|^2$, and is inversely proportional to the magnetic field strength $|\mathbf{B}|$. For an atom positioned at the peak of the Rabi frequency, this displacement would lead to a Stark shift gradient at the atom's position—a situation we explore in Sec. IV.

IV. SINGLE-QUBIT EFFECTS

A. Analytic model

The spatially varying Rabi frequency and Stark shift may be a source of error in single-qubit gates. We investigate their effect by expanding both up to second order in position, $\delta(\hat{x}) = \delta^{(0)} + \delta^{(1)}\hat{x} + \delta^{(2)}\hat{x}^2$ and $\Omega(\hat{x}) = \Omega^{(0)} + \Omega^{(1)}\hat{x} + \Omega^{(2)}\hat{x}^2$. Here, we ignore a global Stark shift imposing $\delta_1(\hat{x}) = -\delta_2(\hat{x})$. We place the ion at x_0 , which sets the Rabi frequency gradient $\Omega^{(1)} = 0$. The Hamiltonian describing the system is then

$$H_3 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \hbar(\delta^{(0)} + \delta^{(1)}\hat{x} + \delta^{(2)}\hat{x}^2)\hat{\sigma}_z + \hbar(\Omega^{(0)} + \Omega^{(2)}\hat{x}^2)\hat{\sigma}_x, \quad (16)$$

where $\hat{x} = l_{\text{ho}}(\hat{a} + \hat{a}^\dagger)$ and $\hat{p} = i(\hbar/2l_{\text{ho}})(\hat{a}^\dagger - \hat{a})$, $\hat{a}$ ($\hat{a}^\dagger$) is the annihilation (creation) operator with $l_{\text{ho}} = \sqrt{\hbar/2m\omega}$ the characteristic length of the harmonic oscillator. The errors associated with qubit-motion coupling due to Rabi frequency curvature $\Omega^{(2)}$ have been studied in previous works [31,45]. We note that errors due to the Stark shift gradient $\delta^{(1)}$ only arise in the nonparaxial case, when the peak of the Stark shift lies off-axis.

We apply two unitary transformations on H_3 (see Appendix B) to eliminate the linear and quadratic qubit-motion coupling induced by the Stark shift components $\delta^{(1)}$ and $\delta^{(2)}$, respectively. Here, we neglect off-resonant motional processes that change the Fock state. The transformed Hamiltonian $\tilde{H}$ in angular frequency units is

$$\tilde{H} = H_{\text{id}} + \kappa_z(\hat{n} + 1/2)\hat{\sigma}_z + \kappa_x(2\hat{n} + 1)\hat{\sigma}_x, \quad (17)$$

where $H_{\text{id}} = \omega(\hat{a}^\dagger \hat{a} + 1/2) + \Omega^{(0)}\hat{\sigma}_x$ is an ideal $\hat{\sigma}_x$ qubit rotation. The second term can be interpreted as the error from squeezing the ion's harmonic motion due to the Stark shift curvature, labeled with error parameter $\kappa_z = 2\delta^{(2)}l_{\text{ho}}^2$. The third term describes σ_x -type errors due to the Rabi frequency curvature and the Stark shift gradient, labeled $\kappa_x = 2\Omega^{(0)}(\delta^{(1)})^2l_{\text{ho}}^2/\omega^2 + \Omega^{(2)}l_{\text{ho}}^2$. The fidelity of the resulting gate is given by [46]

$$\bar{F} = \frac{\sum_l \text{tr}[\hat{U}_{\text{id}}\hat{\sigma}_l^\dagger \hat{U}_{\text{id}}^\dagger \hat{\sigma}_l(\hat{U}_{\text{real}})] + d^2}{d^2(d+1)}, \quad (18)$$

where $\hat{\sigma}_l(\hat{U}_{\text{real}}) \equiv \text{tr}_{\text{FS}}(\hat{U}_{\text{real}}(|n\rangle\langle n| \otimes \hat{\sigma}_l)\hat{U}_{\text{real}}^\dagger)$ is the projector on Fock state $|n\rangle$, and $d = 2$ [16]. The unitaries are $\hat{U}_{\text{id}} = \exp(-iH_{\text{id}}t)$ and $\hat{U}_{\text{real}} = \exp(-i\tilde{H}t)$, and the Fock states are weighted with the Bose-Einstein distribution,

$$P_{\text{th}}(n, \bar{n}) = \frac{\bar{n}^n}{(\bar{n} + 1)^{n+1}}. \quad (19)$$

Here, the average occupation number $\bar{n} = 1/(e^{\frac{\omega\hbar}{k_B T}} - 1)$ is determined by the temperature of the ion crystal, T .

We expand $\bar{F}$ to second order in κ_x and κ_z , and neglect cross terms, to arrive at an analytic expression for the infidelity,

$$1 - \bar{F} \approx \frac{1}{6(\Omega^{(0)})^2}(1 + 8\bar{n}(\bar{n} + 1))(\pi^2\kappa_x^2 + \kappa_z^2), \quad (20)$$

when using a gate time $t_g = \pi/2\Omega^{(0)}$ (the ideal gate time for a $\pi/2$ pulse with H_{id}).

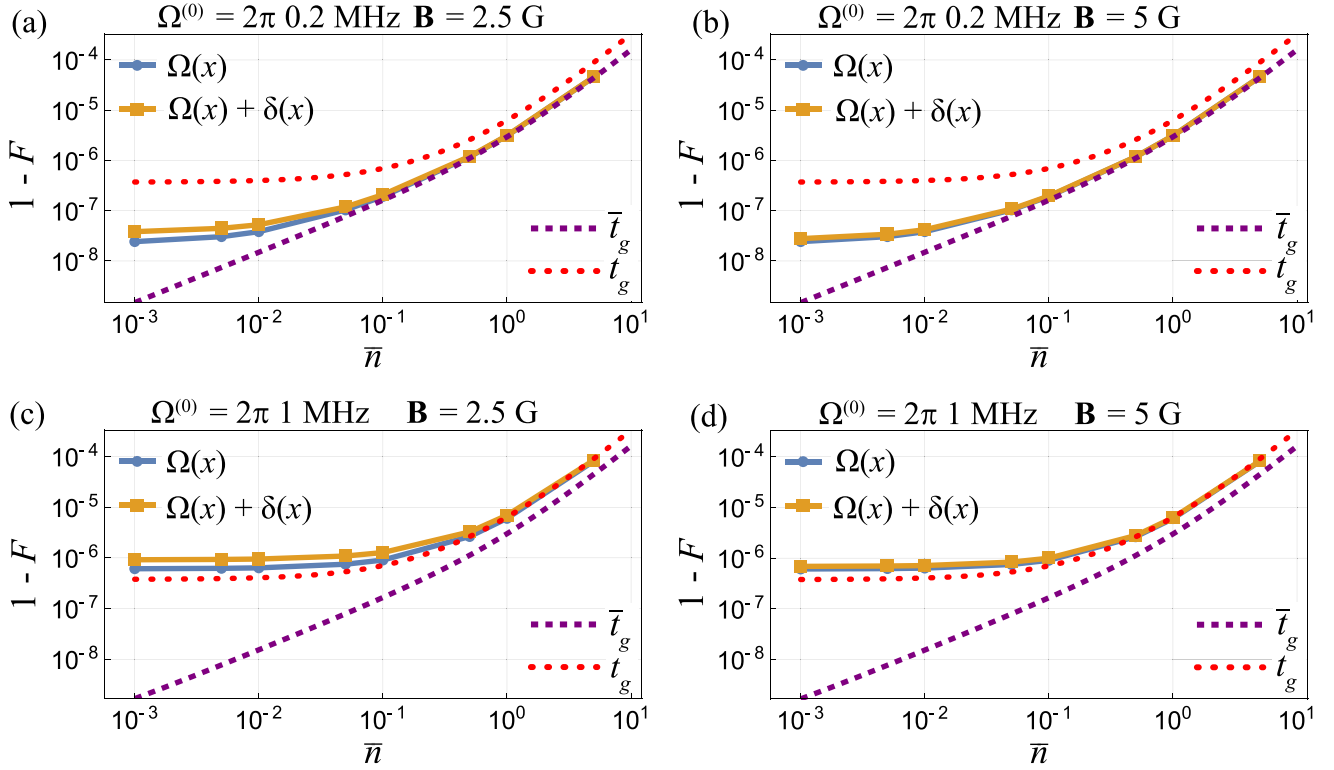


FIG. 4. Single-qubit errors. Simulated infidelity $1 - F$ for a single-qubit $\pi/2$ gate as a function of average occupation $\bar{n}$. We compare simulated errors due to the nonzero components of the Rabi frequency $\Omega(x)$ (blue points) and additionally Stark shift $\delta(x)$ (orange points), with the ion placed at the peak of the Rabi frequency x_0 and using a gate time $\bar{t}_g$. The dashed lines are analytic expressions for the infidelity with a compensated (purple dashed) and uncompensated (red dotted) gate time. We consider Rabi frequency amplitudes $\Omega^{(0)} = 2\pi \cdot 0.2$ and $2\pi \cdot 1$ MHz, and magnetic field strengths $|\mathbf{B}| = 2.5$ and 5 G. Note that the range of temperatures lies below typical Doppler-cooling limits. Decreasing the magnetic field linearly increases the error due to the Stark shift $\delta(x)$, making it more prominent. Increasing the Rabi frequency amplitude increases off-resonant errors, which are excluded in the analytic model, which dominate at low $\bar{n}$.

Considering the physical contributions of the infidelity, the leading error parameter κ_x is dominated by the Rabi frequency curvature $\Omega^{(2)}$ when $\Omega^{(2)}/\Omega^{(0)} > 2(\delta^{(1)})^2/\omega^2$. The ratio of the Rabi frequency curvature to amplitude $\Omega^{(2)}/\Omega^{(0)}$ only changes geometrically, for instance, when the waist is decreased, which increases the Stark shifts quadratically. Consequently, when the trap frequency ω or magnetic field strength is lower, or the beam intensity is higher, the non-paraxial error becomes more significant. For instance, when $\Omega^{(0)} = 2\pi \cdot 1$ MHz, $\mathbf{B} = 2.5$ G, and $\omega = 2\pi \cdot 40$ kHz, the nonparaxial $\delta^{(1)}$ error surpasses the $\Omega^{(2)}$ error, although these parameters are unusual for trapped-ion experiments.

B. Compensated gate time

The κ_x error is an error in the timing of the qubit rotation and can be partially compensated. Assuming we know $\bar{n}$, we can define a new gate time $\bar{t}_g = \pi/2\bar{\Omega}$, where

$$\bar{\Omega} = \Omega^{(0)} + \Omega^{(2)}l_{\text{ho}}^2(2\bar{n} + 1) + (2\Omega^{(0)}(\delta^{(1)})^2l_{\text{ho}}^2/\omega^2)(2\bar{n} + 1) \quad (21)$$

is the thermally averaged Rabi frequency. The first correction, $\Omega^{(2)}l_{\text{ho}}^2(2\bar{n} + 1)$, is due to the Rabi frequency curvature. The second correction, $2\Omega^{(0)}(\delta^{(1)})^2l_{\text{ho}}^2/\omega^2$, is due to the Stark shift gradient, only occurring in the nonparaxial case. Using the

new gate time, we expand Eq. (18) to second order in $\kappa_{x/z}$ to arrive at the infidelity of the compensated gate,

$$1 - \bar{F}_i \approx \frac{2}{3} \cos^2\left(\frac{\pi\gamma}{2}\right) - (1 + 2\bar{n}) \frac{\pi\kappa_x}{3\bar{\Omega}} \sin(\pi\gamma) - \frac{1}{6(\Omega^{(0)})^2} (1 + 8\bar{n}(\bar{n} + 1)) \left(\pi^2 \kappa_x^2 \gamma^2 \cos(\pi\gamma) + \frac{\kappa_z^2}{2} (\cos(\pi\gamma) - 1) + \frac{\pi\kappa_z^2\gamma}{4} \sin(\pi\gamma) \right), \quad (22)$$

where $\gamma = \Omega^{(0)}/\bar{\Omega}$. The analytic expression above allows us to significantly reduce the infidelity without numerical optimization of the gate time. The fidelity calculated with both gate times is compared against numerical simulation in Fig. 4. The dependence of Eq. (22) on the beam waist is considered in Appendix C.

C. Numerical simulation

We compute the fidelity numerically with the Hamiltonian in Eq. (16). In Fig. 4, we show the infidelity evaluated for the parameters in the previous section, with an axial trap frequency $\omega_{\text{ax}} = 2\pi \cdot 0.5$ MHz corresponding to $l_{\text{ho}} = 16$ nm, with two Rabi frequency amplitudes $\Omega^{(0)} = 2\pi \cdot 0.2$ and $2\pi \cdot 1$ MHz, and two magnetic field strengths $|\mathbf{B}| = 2.5$ and 5 G. For the case $\Omega^{(0)} = 2\pi \cdot 1$ MHz and $|\mathbf{B}| = 5$ G, the

field gradients and curvatures at the position of the ion (at $x_0 \sim 108$ nm from the beam center) are $\delta^{(1)} \approx 2\pi 20$ Hz/nm, $\delta^{(2)} \approx 2\pi 0.03$ Hz/nm², and $\Omega^{(2)} \approx 2\pi 2$ Hz/nm², corresponding to fractional error parameters $\kappa_x/\Omega^{(0)} \approx 5 \times 10^{-4}$ and $\kappa_z/\Omega^{(0)} \approx 1 \times 10^{-5}$. We find that $\Omega^{(2)}$ is the dominant error source, as evidenced by the small difference between the solid orange and blue lines, which include and neglect $\delta(x)$, respectively.

Finally, we compare the analytic expression in Eq. (22) with gate time of $\bar{t}_g$ to the numerical results. We attribute the discrepancy between the analytic and the numerical results at larger $\Omega^{(0)}$ to off-resonant processes, which we neglected in our analytic treatment. Finally, we note that the presence of the zero-point energy means that even with the exclusion of off-resonant processes, the infidelity does not tend to 0 as $\bar{n} \rightarrow 0$. In this regime, the performance of the gate is significantly improved by correcting the gate timing as described above (compare the dashed and dotted lines in Fig. 4).

V. TWO-QUBIT EFFECTS

We extend our description to addressing two qubits in an N -ion chain, in order to perform parallel single-qubit operations or two-qubit gates. The system is described by the eigenmodes of the collective motion of the chain, with the position operator for ion k : $\hat{x}_k = \sum_m l_m b_{mk} (\hat{a}_m + \hat{a}_m^\dagger)$ with characteristic length $l_m = \sqrt{\hbar/2m\omega_m}$ for normal mode m , and eigenvector b_{mk} for the k th ion with the m th mode. The errors induced by the nonzero gradient and curvature of the tweezer now couple to each motional mode.

A. Parallel single-qubit gates

Parallel single-qubit gates are described by the Hamiltonian

$$H_4 = H_0 + \Omega^{(0)}(\hat{\sigma}_x^{(i)} + \hat{\sigma}_x^{(j)}) + \Omega^{(2)}(\hat{x}_i^2 \hat{\sigma}_x^{(i)} + \hat{x}_j^2 \hat{\sigma}_x^{(j)}) + \delta^{(1)}(\hat{x}_i \hat{\sigma}_z^{(i)} + \hat{x}_j \hat{\sigma}_z^{(j)}) + \delta^{(2)}(\hat{x}_i^2 \hat{\sigma}_z^{(i)} + \hat{x}_j^2 \hat{\sigma}_z^{(j)}), \quad (23)$$

where $H_0 = \sum_m \omega_m (\hat{a}_m^\dagger \hat{a}_m + 1/2)$. The first explicit term of Hamiltonian (23) describes parallel $\hat{\sigma}_x$ qubit rotations. Performing a Lang-Firsov transformation with unitary $\hat{U}_{\text{LF}} = \exp(\sum_m \zeta_m (b_{mi} \hat{\sigma}_z^{(i)} + b_{mj} \hat{\sigma}_z^{(j)}) (\hat{a}_m^\dagger - \hat{a}_m))$ where $\zeta_m = \delta^{(1)} l_m / \omega_m$ eliminates the linear phonon coupling. Disregarding global energy offsets and off-resonant processes that change the Fock state, the transformed Hamiltonian is

$$\begin{aligned} H_5 &= U_{\text{LF}}^\dagger H_4 U_{\text{LF}} \\ &= H_0 + \Omega^{(0)}(\hat{\sigma}_x^{(i)} + \hat{\sigma}_x^{(j)}) \\ &\quad + \sum_m \left(2\Omega^{(0)} \zeta_m^2 (2\hat{n}_m + 1) (b_{mi}^2 \hat{\sigma}_x^{(i)} + b_{mj}^2 \hat{\sigma}_x^{(j)}) \right. \\ &\quad + \Omega^{(2)} l_m^2 (2\hat{n}_m + 1) (b_{mi}^2 \hat{\sigma}_x^{(i)} + b_{mj}^2 \hat{\sigma}_x^{(j)}) \\ &\quad + \delta^{(2)} l_m^2 (2\hat{n}_m + 1) (b_{mi}^2 \hat{\sigma}_z^{(i)} + b_{mj}^2 \hat{\sigma}_z^{(j)}) \\ &\quad \left. - 2\omega_m \zeta_m^2 b_{bi} b_{bj} \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(j)} \right). \end{aligned} \quad (24)$$

Here, we have used the Baker-Hausdorff lemma to determine the leading-order corrections as in the single-qubit case. H_5

describes (1) parallel single-qubit gates (line 1), (2) coupling between the individual qubits and all motional modes due to the beam gradient and curvature (lines 2–4), and (3) an additional qubit-qubit interaction (line 5). Note that the (2) qubit-motion and (3) qubit-qubit interactions are now site specific due to their dependence on the eigenvectors b_{mi} . With the parameter set used previously, the qubit-qubit interaction is on the Hertz level and thus negligible compared to the individual qubit-motion coupling terms. The fidelity for a certain Fock state configuration $\mathbf{n} = (n_1, n_1, \dots, n_N)$ may be determined numerically, weighted by the probability $P(\mathbf{n}, T) = \prod_m \bar{n}_m^{n_m} / (\bar{n}_m + 1)^{n_m+1}$, but we did not find a simplified approximate analytic expression for this.

B. Mølmer-Sørensen gate

Two-qubit gates can be implemented by amplitude modulating the tweezers with intensity $A(t) = \frac{1}{2}(1 - \cos(\nu t))$, with $\nu = \omega_r + \mu$. Here, the gate uses the radial motion of the ions, with the detuning μ given with respect to the radial trap frequency ω_r . The gate implements interactions $g_r \hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)}$ between ions i and j with $g_r \sim \eta_{mi} \eta_{mj} (\Omega^{(0)})^2 / \mu$, where $\eta_{mj} = b_{mj} \eta = b_{mj} k \sqrt{\hbar/2m\omega_r}$ [47–51]. The errors arise due to the beam gradient and curvature in the axial direction, perpendicular to the action of the gate.

We note that resonant enhancement may occur if ν is close to one of the axial mode frequencies. In this case, qubit-qubit interactions of order $g_{\text{ax}} \sim (\delta^{(1)})^2 l_m^2 / \mu_m$ occur, with μ_m the detuning from the m th axial mode. For the parameters considered here, this amounts to $\lesssim 2\pi 1$ kHz²/μ. For long ion crystals with numerous axial modes, coincidence of ν and ω_m is more likely. This is illustrated in Fig. 5(a), where we show the magnitude of the induced interaction $|g_{\text{ax}}|$ as a function of laser modulation frequency ν for a ten-ion chain with trap frequencies $(\omega_r, \omega_{\text{ax}}) = 2\pi(3.0, 0.5)$ MHz. Note that the interaction strength increases drastically with the Rabi frequency, as $g_{\text{ax}} \propto \Omega^4$. Therefore, a careful choice of parameters will keep the unwanted qubit-qubit interaction to the subhertz level.

We investigate potential gate errors by simulating the Mølmer-Sørensen gate for an $N = 2$ ion chain. The secular trap frequencies are $(\omega_r, \omega_z) = 2\pi(3.0, 0.5)$ MHz resulting in $\eta = 0.056$, and the magnetic field $\mathbf{B} = 2.5$ G lies in the y direction of the tweezers. Using a detuning of $\mu = 2\pi 50$ kHz and $\Omega^{(0)} = 2\pi 228$ kHz for both addressing beams, the gate generates a maximally entangled Bell state in $t_g = 20$ μs. The beam gradient and curvature is $\delta^{(1)} = 2\pi 2.2$ Hz/nm and $\Omega^{(2)} = 2\pi 0.43$ Hz/nm², and the curvature of the Stark shift $\delta^{(2)}$ is negligibly small. We determine the gate fidelity using Eq. (18), both including (denoted by F_{real}) and excluding (denoted by F_{ideal}) the tweezer gradient and curvature. The difference between these two fidelities $\Delta F = F_{\text{real}} - F_{\text{ideal}}$ then describes errors purely due to nonparaxial effects, and we avoid a full analysis on methods to improve the ideal two-qubit gate fidelity (for instance, by pulse shaping [49]). In Fig. 5(b), we plot ΔF against the average thermal occupation $\bar{n}_{\text{com}}$. We note that the cutoff for the three motional modes considered in the simulations is set independently as $\max(n_{\text{com}}, n_{\text{str}}, n_{\text{rad}}) = (12, 8, 12)$. Our results show that the Mølmer-Sørensen gate is robust to the errors considered here,

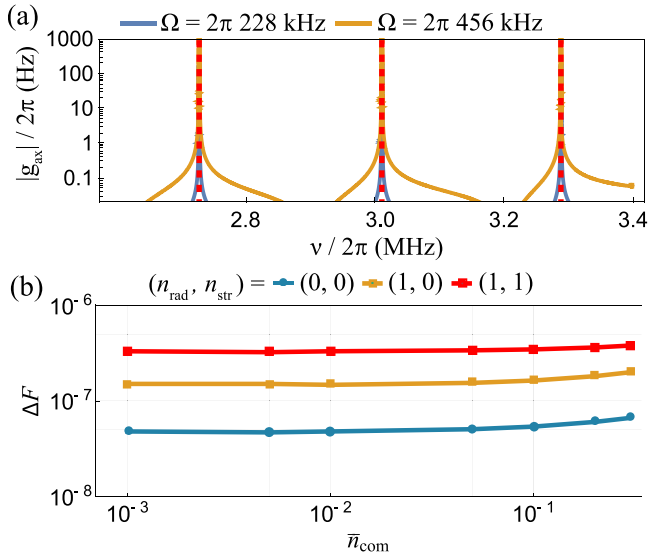


FIG. 5. Two-qubit errors. (a) Magnitude of the axial qubit-qubit interaction $|g_{ax}|$ induced during the Mølmer-Sørensen gate as a function of laser modulation frequency ν . We consider the axial modes (red dashed lines) for a ten-ion chain with trap frequencies $(\omega_r, \omega_z) = 2\pi(3.0, 0.5)$ MHz. The interaction strength is shown for the Rabi frequency used in simulations $\Omega = 2\pi \cdot 228$ kHz (blue) and twice this value $\Omega = 2\pi \cdot 456$ kHz (orange). (b) The fidelity difference ΔF due to the nonzero tweezer gradient $\delta(x)$ and curvature $\Omega(x)$ while performing a Mølmer-Sørensen gate, as a function of average occupation in the axial center-of-mass mode $\bar{n}_{com}$. We consider different Fock state occupations in the radial and axial stretch modes. The gate parameters are $\Omega^{(0)} = 2\pi \cdot 228$ kHz, $\mu = 2\pi \cdot 50$ kHz, and $\eta = 0.056$.

provided that the modes are sufficiently cool. We conclude that the errors considered here are significantly smaller than typical experimental errors due to laser stabilization or beam alignment, and thus do not limit the performance of two-qubit gates in current setups.

VI. DISCUSSION

In this paper, we have considered adverse nonparaxial effects when trapped ions are addressed by tightly focused optical tweezers. The spatial profiles of the atom-light potentials for Gaussian and Laguerre-Gaussian beams are positioned off-axis with respect to the beam intensity. As a result, when an ion is placed at the peak of the Rabi frequency $\Omega(x)$, it experiences a nonzero curvature $\Omega(x)$ and a nonzero gradient of the Stark shift $\delta(x)$. We evaluated the size of the errors resulting from the nonzero curvature and gradient terms while performing single- and two-qubit gates, which manifest as qubit-motion entangling errors. Our numerical simulations, as well as analytic results, show that while the size of the error is strongly dependent on the trapping frequency and the ion temperature, nonparaxial errors are generally very small when using typical experimental parameters. Moreover, suitable choice of laser polarization and magnetic field orientation can be used to partially suppress the errors considered here.

We highlight that nonparaxial effects are potentially more severe when addressing neutral atoms and molecules. The

resulting qubit-motion coupling has been observed as a source of qubit decoherence in Refs. [24,25,52]. For the case of a resonant tweezer, our analysis may be straightforwardly applied to the neutral atom case. Here, the linear qubit-motion coupling parameter $\zeta = \delta^{(1)} l_{ho}/\omega$ would be larger due to the weaker confinement ω compared to ions in a Paul trap. In this case, the single-qubit gate infidelity calculated from Eq. (20) could increase drastically, as $(1 - \bar{F}) \propto \zeta^4$. Note that the coupling also depends on the tweezer parameters, the atomic transition, and the orientation of the magnetic field and polarization. For the case of off-resonant tweezers—for instance, used to confine neutral atoms—nonparaxial effects could also arise. This would depend on the atomic polarizability in the tweezer, and is not considered in this work. Furthermore, other error sources could arise at the scale of the effects considered here. An example of this is intensity fluctuations in the optical tweezer on the spatial scale of the ion's wave packet [53,54]. Finally, nonparaxial effects beyond the universal gate set (single- and two-qubit operations) may arise when simultaneously addressing three or more qubits, but this is beyond the scope of the paper.

In conclusion, the errors considered here lie below the typical thresholds for quantum error correction [55]. Compared to errors due to beam misalignment or laser stabilization, nonparaxial effects are not a limiting factor on current experimental setups. However, at low temperatures and high laser intensities, they can be a distinguishable error source. The effects can be difficult to compensate due to being an inherent feature of the light field. This may be important for the next generation of ion-trap quantum computers, which strive toward lower temperatures and utilize individually addressing, high-intensity beams [56–58]. Furthermore, our theoretical treatment can be applied toward future work, for instance, a detailed study of nonparaxial effects on neutral atoms and molecules [59], and for engineering quantum logic gates that utilize polarization gradients at the center of tightly focused beams, as recently experimentally realized [27,28].

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: GRADIENT AND CURVATURE TERMS

Here, we give analytic expressions for the gradient and curvature terms in H_3 , which cause the considered errors in the text. The Rabi frequency $\Omega(x)$ is well approximated as a displaced Gaussian, and we make a Taylor expansion about the Rabi frequency peak x_0 (where the ion is positioned):

$$\begin{aligned}\Omega(\hat{x}) &\approx \Omega^{(0)} \exp\left(-\frac{(\hat{x} - x_0)^2}{w_0^2}\right) \\ &\approx \Omega^{(0)} \left(1 - \frac{(\hat{x} - x_0)^2}{w_0^2} + \dots\right).\end{aligned}\quad (\text{A1})$$

We identify the coefficient of $\hat{x}^2$ as $\Omega^{(2)} \approx \frac{\Omega^{(0)}}{w_0^2}$. Similarly, the Stark shift is a displaced Gaussian but shifted in the opposite direction and centered at $-x_0$ (as observed in Sec. III). Taylor expanding about the ion's position yields

$$\begin{aligned}\delta(\hat{x}) &\approx \delta^{(0)} \exp\left(-\frac{(\hat{x} + x_0)^2}{w_0^2}\right) \\ &\approx \delta^{(0)} \exp\left(-4x_0^2/w_0^2\right) \left(1 - \frac{4x_0}{w_0^2}(\hat{x} - x_0) - \frac{(w_0^2 - 8x_0^2)}{w_0^4}(\hat{x} - x_0)^2 + \dots\right).\end{aligned}\quad (\text{A2})$$

For larger waists with $w_0^2 \gg x_0^2$ such that $\exp(-4x_0^2/w_0^2) \sim 1$, the gradient and curvature terms simplify to $\delta^{(1)} \sim \frac{4\delta^{(0)}x_0}{w_0^2}$ and $\delta^{(2)} \sim \frac{\delta^{(0)}(w_0^2 - 8x_0^2)}{w_0^4}$. Note that in our case with $w_0 = \lambda$ and $x_0 = \lambda/2\pi$, $\exp(-4x_0^2/w_0^2) = \exp(-\pi^{-2}) \sim 0.9$.

APPENDIX B: HAMILTONIAN TRANSFORMATIONS

We perform a qubit-dependent squeezing transformation on H_3 with unitary

$$\hat{S}(s\hat{\sigma}_z) = \exp\left(\frac{s\hat{\sigma}_z}{2}(\hat{a}^2 - \hat{a}^{\dagger 2})\right). \quad (\text{B1})$$

Using the quadrature transformations $\hat{S}^\dagger(s\hat{\sigma}_z)\hat{a}\hat{S}(s\hat{\sigma}_z) = \hat{a} \cosh(s\hat{\sigma}_z) - \hat{a}^\dagger \sinh(s\hat{\sigma}_z)$ and $\hat{S}^\dagger(s\hat{\sigma}_z)\hat{a}^\dagger\hat{S}(s\hat{\sigma}_z) = \hat{a}^\dagger \cosh(s\hat{\sigma}_z) - \hat{a} \sinh(s\hat{\sigma}_z)$, the motional terms transform as

$$\hat{S}^\dagger(s\hat{\sigma}_z)\hat{x}^2\hat{S}(s\hat{\sigma}_z) = e^{-2s\hat{\sigma}_z}\hat{x}^2, \quad (\text{B2a})$$

$$\hat{S}^\dagger(s\hat{\sigma}_z)\hat{x}\hat{S}(s\hat{\sigma}_z) = e^{-s\hat{\sigma}_z}\hat{x}, \quad (\text{B2b})$$

$$\hat{S}^\dagger(s\hat{\sigma}_z)\hat{p}^2\hat{S}(s\hat{\sigma}_z) = e^{2s\hat{\sigma}_z}\hat{p}^2. \quad (\text{B2c})$$

The squeezed Hamiltonian is

$$\begin{aligned}\tilde{H} &= \hat{S}^\dagger(s\hat{\sigma}_z)H_3\hat{S}(s\hat{\sigma}_z) \\ &= \frac{1}{2m}e^{2s\hat{\sigma}_z}\hat{p}^2 + \frac{1}{2}e^{-2s\hat{\sigma}_z}m\omega^2\hat{x}^2 \\ &\quad + \hbar(\delta^{(0)} + \delta^{(1)}e^{-s\hat{\sigma}_z}\hat{x} + \delta^{(2)}e^{-2s\hat{\sigma}_z}\hat{x}^2)\hat{\sigma}_z \\ &\quad + \hbar\hat{S}^\dagger(s\hat{\sigma}_z)\hat{\Omega}\hat{\sigma}_x\hat{S}(s\hat{\sigma}_z).\end{aligned}\quad (\text{B3})$$

We define a qubit-dependent frequency $\tilde{\omega} = \sqrt{\omega^2 + \frac{2\delta^{(2)}\hbar}{m}}\hat{\sigma}_z$, which absorbs $\delta^{(2)}$ into the ion's harmonic motion. By first-order Taylor expansion, $\tilde{\omega} \approx \omega + (\delta^{(2)}l_{\text{ho}}^2)\hat{\sigma}_z$. The Rabi frequency components are denoted by $\hat{\Omega} = \Omega^{(0)} + \Omega^{(2)}\hat{x}^2$. In

terms of creation and annihilation operators, the Hamiltonian (in angular frequency units) is

$$\begin{aligned}\tilde{H} &= -\frac{e^{2s\hat{\sigma}_z}}{4}\omega(\hat{a}^{\dagger 2} + \hat{a}^2 - 2\hat{a}^\dagger\hat{a} - 1) \\ &\quad + \frac{e^{-2s\hat{\sigma}_z}}{4}\frac{\tilde{\omega}^2}{\omega}(\hat{a}^{\dagger 2} + \hat{a}^2 + 2\hat{a}^\dagger\hat{a} + 1) \\ &\quad + (\delta^{(0)} + \delta^{(1)}e^{-s\hat{\sigma}_z}l_{\text{ho}}(\hat{a} + \hat{a}^\dagger))\hat{\sigma}_z \\ &\quad + \hat{S}^\dagger(s\hat{\sigma}_z)\hat{\Omega}\hat{\sigma}_x\hat{S}(s\hat{\sigma}_z).\end{aligned}\quad (\text{B4})$$

We recover the harmonic oscillator with frequency $\tilde{\omega}$ by choosing the squeezing parameter $s = \delta^{(2)}l_{\text{ho}}^2/\omega$ as a dimensionless measure of the Stark shift curvature. The Hamiltonian is then

$$\begin{aligned}\tilde{H} &= \tilde{\omega}(\hat{a}^\dagger\hat{a} + 1/2) + \delta^{(0)}\hat{\sigma}_z \\ &\quad + \delta^{(1)}e^{-s\hat{\sigma}_z}x_0(\hat{a} + \hat{a}^\dagger)\hat{\sigma}_z \\ &\quad + \hat{S}^\dagger(s\hat{\sigma}_z)\hat{\Omega}\hat{\sigma}_x\hat{S}(s\hat{\sigma}_z).\end{aligned}\quad (\text{B5})$$

Similarly, the linear motion term can be transformed through a qubit-dependent Lang-Firsov transformation with unitary

$$\hat{D}(\zeta\hat{\sigma}_z) = \exp(\zeta\hat{\sigma}_z(\hat{a}^\dagger - \hat{a})), \quad (\text{B6})$$

with quadrature transformations $\hat{D}^\dagger(\zeta\hat{\sigma}_z)\hat{a}\hat{D}(\zeta\hat{\sigma}_z) = \hat{a} - \zeta\hat{\sigma}_z$ and $\hat{D}^\dagger(\zeta\hat{\sigma}_z)\hat{a}^\dagger\hat{D}(\zeta\hat{\sigma}_z) = \hat{a}^\dagger - \zeta^*\hat{\sigma}_z$. The Hamiltonian becomes

$$\begin{aligned}\tilde{H} &= \tilde{\omega}(\hat{a}^\dagger\hat{a} + 1/2 - \zeta\hat{\sigma}_z(\hat{a} + \hat{a}^\dagger) + \zeta^2) \\ &\quad + \delta^{(0)}\hat{\sigma}_z + \delta^{(1)}e^{-s\hat{\sigma}_z}x_0(\hat{a} + \hat{a}^\dagger)\hat{\sigma}_z \\ &\quad - 2\delta^{(1)}e^{-s\hat{\sigma}_z}x_0\zeta \\ &\quad + \hat{D}^\dagger(\zeta\hat{\sigma}_z)\hat{S}^\dagger(s\hat{\sigma}_z)\hat{\Omega}\hat{\sigma}_x\hat{S}(s\hat{\sigma}_z)\hat{D}(\zeta\hat{\sigma}_z),\end{aligned}\quad (\text{B7})$$

when ζ is real. The linear motion terms cancel out by choosing the displacement parameter $\zeta = \delta^{(1)}l_{\text{ho}}/\omega$ to be a dimensionless measure of the Stark shift gradient. The Hamiltonian simplifies to

$$\begin{aligned}\tilde{H} &= \tilde{\omega}(\hat{a}^\dagger\hat{a} + 1/2) - \tilde{\omega}\zeta^2 + \delta^{(0)}\hat{\sigma}_z \\ &\quad + \hat{D}^\dagger(\zeta\hat{\sigma}_z)\hat{S}^\dagger(s\hat{\sigma}_z)\hat{\Omega}\hat{\sigma}_x\hat{S}(s\hat{\sigma}_z)\hat{D}(\zeta\hat{\sigma}_z).\end{aligned}\quad (\text{B8})$$

Disregarding energy offsets that do not contribute to qubit-motion coupling, like $\delta^{(0)}\hat{\sigma}_z$, which can be fixed by the laser frequency, the Hamiltonian is

$$\begin{aligned}\tilde{H} &= \tilde{\omega}(\hat{a}^\dagger\hat{a} + 1/2) \\ &\quad + \hat{D}^\dagger(\zeta\hat{\sigma}_z)\hat{S}^\dagger(s\hat{\sigma}_z)\hat{\Omega}\hat{\sigma}_x\hat{S}(s\hat{\sigma}_z)\hat{D}(\zeta\hat{\sigma}_z).\end{aligned}\quad (\text{B9})$$

The first term describes the ion's motion as a modified harmonic oscillator with frequency $\tilde{\omega}$. The second term describes the ion-laser coupling acted on by squeeze and displacement operators dependent on the qubit state of the ion. We calculate the effect of these transformations using the Baker-Hausdorff (BH) lemma, which gives corrections to the Rabi frequency $\hat{\Omega} = \Omega^{(0)} + \Omega^{(2)}\hat{x}^2$. First, evaluating the Rabi frequency amplitude $\Omega^{(0)}$ and disregarding off-resonant processes that

change the Fock state,

$$\begin{aligned} & \hat{D}^\dagger(\zeta \hat{\sigma}_z) \hat{S}^\dagger(s \hat{\sigma}_z) (\Omega^{(0)} \hat{\sigma}_x) \hat{S}(s \hat{\sigma}_z) \hat{D}(\zeta \hat{\sigma}_z) \\ &= \Omega^{(0)} \left(1 + 2\zeta^2(2\hat{n} + 1) + \frac{s\zeta}{2}(2\hat{n} + 1) + O(\hat{n}^2) \right) \hat{\sigma}_x. \end{aligned} \quad (\text{B10})$$

We neglect terms higher than the first correction proportional to ζ^2 (which are strongly suppressed as $s \ll \zeta$).

We then calculate the effect of the squeeze and displacement transformation on the Rabi frequency curvature $\Omega^{(2)} \hat{x}^2$. Again, using the BH lemma, we find

$$\begin{aligned} & \hat{D}^\dagger(\zeta \hat{\sigma}_z) \hat{S}^\dagger(s \hat{\sigma}_z) (\Omega^{(2)} \hat{x}^2 \hat{\sigma}_x) \hat{S}(s \hat{\sigma}_z) \hat{D}(\zeta \hat{\sigma}_z) \\ &= \Omega^{(2)} l_{\text{ho}}^2 (2\hat{n} + 1) \left(1 + 2\zeta^2(2\hat{n} + 1) \right. \\ & \quad \left. + \frac{s\zeta}{2}(2\hat{n} + 1) + O(\hat{n}^2) \right) \hat{\sigma}_x. \end{aligned} \quad (\text{B11})$$

Here, we neglect all higher-order terms than the first, as these are found to be negligible with our parameter set. Inserting Eqs. (B10) and (B11) into Eq. (B9), the Hamiltonian may be written in terms of the physical parameters as

$$\begin{aligned} \tilde{H} &= \omega(\hat{a}^\dagger \hat{a} + 1/2) + \Omega^{(0)} \hat{\sigma}_x + 2\delta^{(2)} l_{\text{ho}}^2 (\hat{n} + 1/2) \hat{\sigma}_z \\ &+ \left((2\Omega^{(0)} (\delta^{(1)})^2 l_{\text{ho}}^2 / \omega^2) (2\hat{n} + 1) + \Omega^{(2)} l_{\text{ho}}^2 (2\hat{n} + 1) \right) \hat{\sigma}_x. \end{aligned} \quad (\text{B12})$$

In the text, this is simplified to

$$\tilde{H} = H_{\text{id}} + \kappa_z (\hat{n} + 1/2) \hat{\sigma}_z + \kappa_x (2\hat{n} + 1) \hat{\sigma}_x, \quad (\text{B13})$$

where

$$H_{\text{id}} = \omega(\hat{a}^\dagger \hat{a} + 1/2) + \Omega^{(0)} \hat{\sigma}_x, \quad (\text{B14})$$

$$\kappa_z = 2\delta^{(2)} l_{\text{ho}}^2, \quad (\text{B15})$$

$$\kappa_x = 2\Omega^{(0)} (\delta^{(1)})^2 l_{\text{ho}}^2 / \omega^2 + \Omega^{(2)} l_{\text{ho}}^2. \quad (\text{B16})$$

In our analytic treatment, we have neglected off-resonant processes that change the Fock state n . In Fig. 4, we see that

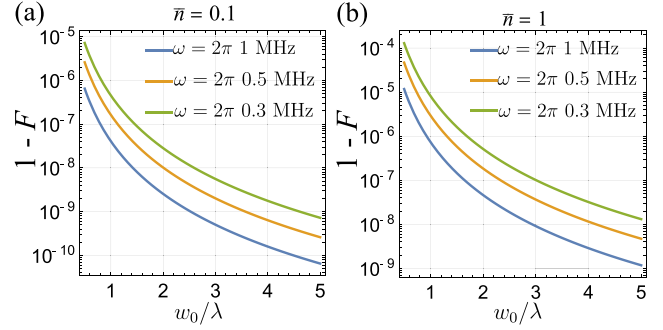


FIG. 6. Analytic infidelity from Eq. (22) for the single-qubit gate as a function of tweezer waist w_0 , with different trap frequencies ω . Here, $\Omega^{(0)} = 2\pi \cdot 0.2$ MHz, $\mathbf{B} = 2.5$ G, and the ion temperature is fixed at (a) $\bar{n} = 0.1$ and (b) $\bar{n} = 1$.

off-resonant terms become significant when $\bar{n} \ll 1$ or $\Omega \gg \omega$, by comparing the analytic and numerical curves. We note that instead of using the BH lemma, we can utilize the expression for the overlap of a squeezed-displaced Fock state from Ref. [60]. The overlap gives the transformed Rabi frequency for a given Fock state, $\Omega^{(0)} \langle -\zeta, -s, n | \zeta, s, n \rangle \hat{\sigma}_x$, which is well approximated by the first few terms of the BH lemma when ζ and s are small. The overlap also allows the calculation of off-resonant processes that change the Fock state $n \rightarrow m$, by $\Omega^{(0)} \langle -\zeta, -s, m | \zeta, s, n \rangle \hat{\sigma}_x$. This could be of interest, for instance, to find tweezer parameters that specifically drive the sidebands $n \rightarrow n \pm 1$ or generate anharmonic potentials.

APPENDIX C: DEPENDENCE ON TWEEZER WAIST

Here, we consider how the single qubit infidelity calculated in Sec. IV varies with the beam waist w_0 in Fig. 6. As the waist increases, nonparaxial errors become practically negligible. However, we note that increasing the waist is not always a valid solution in experimental setups, for instance, when addressing multiple ions in a chain. Here, a larger waist can cause crosstalk with adjacent ions. In this case, one could find an optimal tweezer waist that minimizes both crosstalk and nonparaxial effects. A more straightforward solution may be to use a magnetic field and polarization orientation that suppresses the nonparaxial error.

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