# Entangling ions in arrays of microscopic traps

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We consider a system of particles in an array of microscopic traps, coupled to each other via electrostatic interaction, and pushed by an external state-dependent force. We show how to implement a two-qubit quantum gate between two such particles with a high fidelity.

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## I. INTRODUCTION

The possibilities offered by quantum mechanical systems for efficient information processing have stimulated the rise of an entire field of research in recent years [1]. Quantum protocols for secure communication over long distances have been devised and demonstrated. Quantum algorithms for efficient solution of problems believed to be intractable on classical computers have been developed. However, while quantum communication is already approaching the stage of real-world applications, quantum computation still remains at a less advanced level, as far as physical implementation is concerned. Different systems have been proposed as candidates for this purpose [2], but nobody can yet tell what will turn out to be a viable solution. Indeed, in a few cases quantum computation building blocks—single- and two-qubit operations—have already been demonstrated experimentally. In principle, these ingredients are universal—they are sufficient to build an arbitrary unitary transformation over $N$ qubits (i.e., any quantum computation). But in order to perform useful computations in a real environment inducing decoherence, fault tolerance is also required. This implies, e.g., nested redundant coding for real-time error correction [3], and requires an error probability for elementary operations below a certain threshold (of the order of $10^{-4}$). Hence the need for proposals allowing for handling a bigger number of qubits at a lower decoherence rate and with faster and more reliable gate operations—in a word, enabling scalability of the system.

We propose to use quantum optical systems in periodic microscopic potentials. This is meant to combine the good isolation and precise control by laser fields achievable in quantum optics, with the ability—usually associated with semiconductor technology—to manufacture periodic structures to generate modulated fields on a microscopic scale. The general concept of our proposal is to encode the logical states of each qubit into two internal states of a particle (neutral atom or ion). Single-qubit operations are obtained as Rabi rotations by applying resonant laser fields. Two-qubit gates are performed by inducing a state-dependent interaction over a certain time, making the particles acquire a conditional phase shift depending on their logical states. These, however, in a real situation are coupled to other external degrees of freedom. This can lead to different kinds of imperfection. On one hand, the external state after gate operation may not be exactly the same as before. On the other hand, the conditional phase shift will also depend on the external state: if this is mixed, only an imprecise phase determination will be possible. These facts affect the gate fidelity, which is defined by comparing the desired effect of the gate with the actual evolution that can be obtained in the laboratory. We have already proposed several schemes, based on different interactions—collisional interactions between neutral atoms in optical lattices [4] and magnetic microtraps [5], or dipole-dipole interactions between Rydberg-excited atoms [6]. Here we describe in detail a scheme that was earlier proposed in [7]. It relies on ions stored in an array of microscopic traps [8]. The idea is to displace the motional wave function of each ion by a small amount, conditional on its internal state. This can be effected via external (e.g., laser) fields. The electrostatic interaction energy thus depends on the internal states of both ions, and a state-selective two-particle phase shift can be obtained. This scheme has a number of advantages with respect to the previous ion trap proposal [9], which we will discuss later.

According to the model described above, in this paper we deal with the conditional dynamics of two charged particles, trapped in separate harmonic wells, interacting via electrostatic repulsion and under the influence of an external state-dependent force, which can be generated, e.g., by an off-resonant laser standing wave [7]. The goal is to implement a phase gate between the two qubits (Sec. II), i.e., to transform their initial state by inducing a certain phase onto each of its components. The ideal transformed state so defined has to be compared to the one that can be obtained by means of a realistic Hamiltonian, coupling the particles' internal and external degrees of freedom (Sec. III). With this aim, we consider first a one-dimensional classical model for the motion (Sec. IV). We solve the equations of motion for each combination of logical states separately, and define in each case a two-particle phase as the integral over time of the interaction energy. These phases define the evolved internal state, to be compared eventually with the ideal state we aim to obtain. The fidelity of gate operation is evaluated, in this classical model, as the overlap between the real and the ideal states, averaged over different starting conditions according to a thermal probability distribution for the initial oscillation energies. The outcome is a series expansion for the temperature dependence of the fidelity, of which we give the first terms explicitly. The full three-dimensional quantum mechanical

 

calculation follows the same path (Sec. V), except for two points. First, the two-particle phases are now given directly by the Schrödinger equation and not defined *ad hoc* as before. Second, the fidelity is evaluated by tracing out the external variables of a density matrix representing a mixed thermal quantum state. We calculate perturbative corrections arising from multipole terms in the Coulomb potential, and show how to suppress lowest-order corrections to the fidelity by means of an intermediate $\pi$ rotation on the qubits, thus achieving an improvement by several orders of magnitude.

## II. A QUANTUM PHASE GATE

We want to implement quantum logic between particles stored in an array of microscopic traps. The qubits' logical states $|0\rangle$ and $|1\rangle$ are encoded into the particles' internal states. One basic building block toward multiqubit entanglement operations is the phase gate between two qubits—a transformation that rotates by a certain phase just one component of the logical states:

$$\begin{aligned} |0\rangle|0\rangle &\rightarrow |0\rangle|0\rangle, \\ |0\rangle|1\rangle &\rightarrow |0\rangle|1\rangle, \\ |1\rangle|0\rangle &\rightarrow |1\rangle|0\rangle, \\ |1\rangle|1\rangle &\rightarrow e^{i\vartheta}|1\rangle|1\rangle. \end{aligned} \tag{2.1}$$

When $\vartheta=\pi$, this is equivalent—up to single-qubit rotations—to a controlled-NOT gate. Ideally, this would be accomplished by means of a state-dependent interaction of the form

$$H_{\rm int}=\Delta E(t)|1\rangle_1\langle 1|\otimes|1\rangle_2\langle 1|, \tag{2.2}$$

acting over a time $\tau$ such that

$$\int_0^\tau \Delta E(t')dt'=\vartheta. \tag{2.3}$$

However, it is not straightforward to realize in practice an interaction between two particles that couples only their internal states—other degrees of freedom, for instance, the motional ones, are likely to be affected. Therefore our goal is to approximate the ideal transformation Eq. (2.1) by means of a conditional dynamics for two particles, making them acquire the phase $\vartheta$ if and only if they are both in the internal state $|1\rangle$, and eventually leaving the external degrees of freedom essentially unaffected. This is described by a Hamiltonian of the form

$$H(t,\mathbf{x}_1,\mathbf{x}_2)=\sum_{\alpha,\beta=0}^{1} H^{\alpha\beta}(t,\mathbf{x}_1,\mathbf{x}_2)|\alpha\rangle_1\langle\alpha|\otimes|\beta\rangle_2\langle\beta|, \tag{2.4}$$

where $\mathbf{x}_j$ denotes the external degrees of freedom of particle $j$, and the explicit time dependence indicates that we can switch on and off a suitable interaction in order to obtain the desired effect. To evaluate the performance of our scheme, we have to compare the case of an ideal gate, as given by Eq. (2.1), with the gate that can actually be realized by the physical process described by Eq. (2.4). The figure of merit is the minimum fidelity $F$, given by

$$F=\min_{\chi} {\rm tr}_{\rm ext}\langle\chi'|\sigma'|\chi'\rangle, \tag{2.5}$$

where $\mathrm{tr}_{\rm ext}$ denotes the trace over the external degrees of freedom, $|\chi\rangle\equiv\Sigma_{\alpha\beta}c_{\alpha\beta}|\alpha\rangle_1|\beta\rangle_2$ is a generic two-ion internal state, $|\chi'\rangle$ is the state obtained from $|\chi\rangle$ via the transformation Eq. (2.1), and $\sigma'$ is the total density matrix, including external degrees of freedom, after the evolution dictated by the Hamiltonian Eq. (2.4), starting from an initial state

$$\sigma\equiv\rho_1(t_0)\otimes\rho_2(t_0)\otimes|\chi\rangle\langle\chi|, \tag{2.6}$$

where $\rho_j(t_0)$ is the external state of particle $j$ at the initial time $t_0$. Ideally, to achieve the optimal fidelity $F=1$, we need the external degrees of freedom to factorize after the gate operation, and the evolution operator

$$U(t,t_0)\equiv T\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} H(t',\mathbf{x}_1,\mathbf{x}_2)dt'\right\} \tag{2.7}$$

to have the sole effect of inducing a two-particle phase $\varphi^{\alpha\beta}$ depending on the internal state of both ions, plus single-particle phases due to the kinetic energy associated with the trap displacement. The latter can be undone by means of single-qubit rotations (see Appendix B 1), leaving us with the gate phase

$$\vartheta=\varphi^{00}-\varphi^{01}-\varphi^{10}+\varphi^{11}. \tag{2.8}$$

In a real situation, the starting point will rather be a mixed state corresponding to a thermal distribution over the external energy eigenstates. In other words, at nonzero temperatures there will be a finite probability that each particle starts in an excited motional state, leading in general to different phases, which cannot be experimentally controlled and easily undone by single-qubit rotations. Therefore the fidelity is expected to decrease with temperature, as we are going to show quantitatively in the next sections, both in a classical model for the particles' motion and in a fully quantum framework.

## III. CONDITIONAL DYNAMICS

We consider $N$ ions, trapped at positions denoted by ($c$ numbers) $\overline{\mathbf{r}_i}$ $(1\leqslant i\leqslant N)$. For simplicity, we take the trapping potentials for all ions to be harmonic, with the same frequency $\omega$ along every spatial direction. Our results can be straightforwardly generalized to inhomogeneous trap arrays with anisotropic confinement. Moreover, each ion is assumed to be subject to a time-varying force $\mathbf{F}_i(t)$, depending on its internal state $\alpha_i\in\{0,1\}$ as in Eq. (2.4). The Hamiltonian is

$$H=\sum_{i=1}^{N} H_i+\sum_{i<j}^{N} H_{ij}, \tag{3.1}$$

where

$$H_i \equiv \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} m\omega^2 (\mathbf{r}_i - \overline{\mathbf{r}}_i)^2 - \mathbf{F}_i(t)\cdot\mathbf{r}_i , \tag{3.2a}$$

$$H_{ij} \equiv \frac{q_e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{3.2b}$$

In the following, we will focus on two-particle dynamics. We assume the external force to have the same strength on both ions, i.e., to depend only on the internal state of each particle:

$$\mathbf{F}_i(t) = \sum_{\alpha=0}^{1} |\alpha\rangle_i\langle\alpha| \otimes \mathbf{F}^{\alpha}(t). \tag{3.3}$$

We can rewrite the Hamiltonian in Eq. (2.4) as

$$H^{\alpha_1\alpha_2}(t,\mathbf{x}_1,\mathbf{x}_2) = \sum_{i=1}^{2} \left\{ \frac{\mathbf{p}_i^2}{2m} + \frac{m\omega^2}{2}[\mathbf{x}_i - \mathbf{x}^{\alpha_i}(t)]^2 - \frac{\mathbf{F}^{\alpha_i}(t)^2}{2} \right\} + \frac{q_e^2}{4\pi\varepsilon_0} \frac{1}{|\mathbf{d} + \mathbf{x}_2 - \mathbf{x}_1|}, \tag{3.4}$$

where we have defined $\mathbf{x}_1 \equiv \mathbf{r}_1 + \mathbf{d}/2$, $\mathbf{x}_2 \equiv \mathbf{r}_2 - \mathbf{d}/2$, $\mathbf{x}^{\alpha}(t) \equiv \mathbf{F}^{\alpha}(t)/(m\omega^2)$, and $\mathbf{d}$ is the equilibrium interparticle separation. We assume the external force to act along its direction, and we choose the simple state dependence $\mathbf{F}^{\alpha}(t) \equiv (\alpha\hbar\omega\mathcal{F}(t)/a_{\omega},0,0)$. Here $a_{\omega} \equiv \sqrt{\hbar/m\omega}$ is the quantum harmonic oscillator ground-state width. Hence the adimensional quantity $\mathcal{F}(t)$ represents the displacement, in units of $a_{\omega}$, induced by the force on the trap minimum for ion $i$, if it is in internal state $|1\rangle_i$: indeed, we have $\mathbf{x}^{\alpha}(t) = \alpha a_{\omega}(\mathcal{F}(t),0,0)$. With the above choice for the state dependence of the force, the term in square brackets on the right-hand side of Eq. (3.4) will not contribute to the gate phase Eq. (2.8), since the corresponding terms cancel each other in the sum $\Sigma_{\alpha,\beta}(-1)^{\alpha+\beta}\varphi^{\alpha\beta}$. Since the interaction depends only on the distance between the particles, it will affect only the relative motion. Therefore we can study the problem in the coordinate system where the relative motion is decoupled from the center-of-mass degrees of freedom. The Hamiltonian can be rewritten (see Appendix A 1) as $H(t) = H_R(t) + H_r(t)$, where

$$H_R(t) = H_R^0 - \mathbf{F}(t)\cdot\left(\mathbf{R} + \frac{\overline{\mathbf{r}_1} + \overline{\mathbf{r}_2}}{2}\right), \tag{3.5a}$$

$$H_r(t) = H_r^0 - \mathbf{f}(t)\cdot(\mathbf{r} + \mathbf{d}) + H_1 . \tag{3.5b}$$

Here, $H_R^0$ and $H_r^0$ contain three-dimensional harmonic potentials, and describe also nonadiabatic effects arising when $\omega\tau \sim 1$. In particular, $H_r^0$ incorporates terms arising from the interaction up to the order $(a_{\omega}/d)^2$. $H_1$ entails the higher-order multipole contributions.

## IV. A CLASSICAL MODEL

We first treat the ions' motion classically, i.e., we regard them as point particles following well-defined trajectories

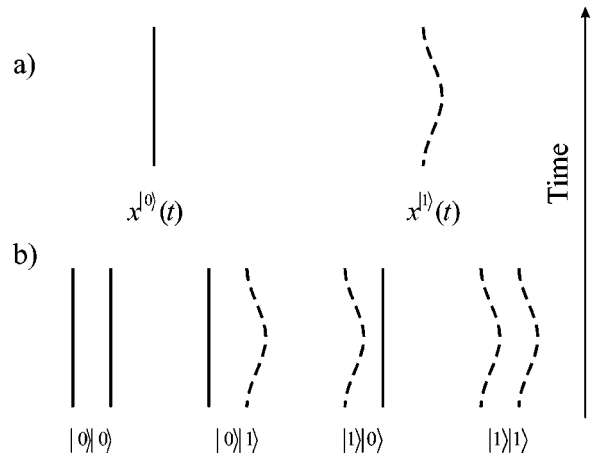


FIG. 1. Gate operation scheme in a classical picture. Above: selective trap displacement for the two different internal states. Below: schematics of the four different Hamiltonians for each combination of internal states.

dictated by the state-dependent trapping potential and by the repulsive electrostatic force. Without loss of generality, we can take the $x$ axis parallel to $\mathbf{d}$. We will study the one-dimensional problem of the motion along that direction, denoting by italic letters the first Cartesian component of the vectors defined in the previous section. The initial state of the system is described by the internal quantum state

$$|\chi_{\mathrm{cl}}(t_0)\rangle \equiv \sum_{\alpha,\beta=0}^{1} c_{\alpha\beta}|\alpha\rangle_1|\beta\rangle_2 \tag{4.1}$$

and by the external classical trajectories $x_i^{\alpha\beta}(t)$ of the two ions, dictated by the Hamiltonian Eq. (2.4). Here, by $\alpha \rightleftharpoons \alpha_1$ ($\beta \rightleftharpoons \alpha_2$) we mean the internal state of the first (second) particle. To find the trajectories for all values of $\alpha$ and $\beta$, we have to solve four distinct classical two-particle equations of motion, each describing the dynamics for one of the possible combinations of internal states, as depicted in Fig. 1. Once we have done that, we can evaluate the Coulomb interaction energy

$$V^{\alpha\beta}(t) \equiv \frac{q_e^2}{4\pi\varepsilon_0} \frac{1}{|d + x_2^{\alpha\beta}(t) - x_1^{\alpha\beta}(t)|} = \frac{q_e^2}{4\pi\varepsilon_0 d} \sum_{n=0}^{\infty} \left[\frac{x_1^{\alpha\beta}(t) - x_2^{\alpha\beta}(t)}{d}\right]^n . \tag{4.2}$$

We then define the evolved internal state as

$$|\chi_{\mathrm{cl}}(t)\rangle \equiv \sum_{\alpha\beta} c_{\alpha\beta}|\alpha\rangle|\beta\rangle e^{i\varphi_{\mathrm{cl}}^{\alpha\beta}}, \tag{4.3}$$

where

$$\varphi_{\mathrm{cl}}^{\alpha\beta} \equiv -\frac{1}{\hbar}\int_{t_0}^{t} V^{\alpha\beta}(t')dt'. \tag{4.4}$$

Now we make the following assumptions: (i) the force acts slowly over the harmonic oscillator time scale $\omega^{-1}$, i.e., $|\dot{\mathcal{F}}| \ll \omega$; (ii) it induces a displacement of the order of the single-trap harmonic oscillator length $a_\omega$; (iii) the latter is much smaller than the distance between the traps, i.e., $a_\omega \ll d$; (iv) the amplitude of the intrawell oscillations (if any) is negligible with respect to the interwell distance, i.e., $E_i \ll m\omega^2 d^2/2$. The first three conditions can be fulfilled by construction; the last one in principle requires the motion to be cooled. Assumption (i) amounts to neglecting nonadiabatic terms in the trajectories (e.g., the sloshing motion excited by the trap displacement). On the other hand, when the last three assumptions hold, we can consider, to a first approximation, the intrawell motion to be essentially unaffected by the higher-order multipole terms in the expansion of the Coulomb interaction, Eq. (4.2). This approximation is not easy to check classically, since the exact trajectories cannot be computed analytically. We will test its validity in second-order perturbation theory, in the context of the quantum mechanical treatment (see Appendix B 4).

### A. Starting conditions

The initial classical motional state, at $t=t_0$, can be either the ground state, described by the initial conditions $x_i(t_0) = \dot{x}_i(t_0) = 0$, or an excited state, described by oscillations of each ion inside its trap with an energy $E_i$ $(i=1,2)$, i.e., by the initial conditions

$$x_i(t_0) = \Delta x_i^{E_i}(t_0) \equiv \sqrt{\frac{2E_i}{m\tilde{\omega}^2}} \cos[\tilde{\omega}(t_0 - t_i)], \quad (4.5a)$$

$$\dot{x}_i(t_0) = -\sqrt{\frac{2E_i}{m}} \sin[\tilde{\omega}(t_0 - t_i)] \quad (4.5b)$$

(of course, the former is a particular case of the latter, for $E_1 = E_2 = 0$). Here, $\tilde{\omega}$ is a corrected trap frequency, taking into account up to quadratic terms in the Coulomb potential—i.e., up to $n=2$ in Eq. (4.2)—namely, $\tilde{\omega} \equiv \omega\sqrt{1+\epsilon/2}$, where

$$\epsilon \equiv \frac{q_e^2}{\pi\varepsilon_0 m\omega^2 d^3} \quad (4.6)$$

is essentially twice the ratio of the Coulomb energy $q_e^2/(4\pi\varepsilon_0 d)$ and the energy of the second ion with respect to the first trap $m\omega^2 d^2/2$. Under the approximations discussed above, we can write the trajectories $x_i^{\alpha\beta}(t)$ as

$$x_i^{\alpha_1\alpha_2}(t) \approx x_i^{\alpha_i}(t) + \Delta x_i^{E_i}(t) \quad (4.7)$$

at all times. The situation is depicted in Fig. 2. Note that we are treating classically the particle motion, but not the internal state: so the ions are allowed to be in a superposition of the available logical states, i.e., to oscillate according to two different trapping potentials, as seen in Fig. 2.

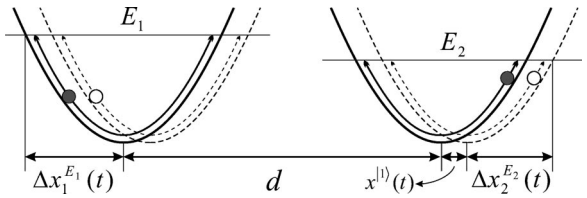


FIG. 2. Gate operation dynamics for two classical particles oscillating with energies $E_i$. The state-selective trap displacements $x^{\alpha_i}(t)$ and the intrawell oscillations $\Delta x_i^{E_i}(t)$ are shown.

### B. Gate phases

We can write the phases Eq. (4.4) as

$$\varphi_{\rm cl}^{\alpha\beta} = \phi_{\rm cl}^{\alpha\beta} + \delta\phi^{\alpha\beta}, \quad (4.8)$$

where $\phi_{\rm cl}^{\alpha\beta}$ is the ground-state contribution and $\delta\phi^{\alpha\beta}$ is the correction due to motional excitations. To evaluate the various contributions explicitly under the above approximations, we now need only specify the time dependence of the trap displacement. We choose the Gaussian form

$$\mathcal{F}(t) \equiv \xi e^{-(t/\tau)^2}. \quad (4.9)$$

Let us first consider the case where both particles are in their motional ground state. We insert Eq. (4.7) for $E_i = 0$, through Eq. (4.2), into Eq. (4.4), and obtain

$$\phi_{\rm cl}^{\alpha\beta} = -(\alpha-\beta)^2 \sqrt{\frac{\pi}{8}} \xi^2 \epsilon \tilde{\omega}\tau \sum_{n=0}^{\infty} \frac{[(\alpha-\beta)\xi a_{\tilde{\omega}}/d]^{n-1}}{\sqrt{2(n+1)}}. \quad (4.10)$$

In the evaluation of the ground-state phase $\phi_{\rm cl}^{\alpha\beta}$, Eq. (4.10), the complete Coulomb potential Eq. (4.2) has been taken into account. When we evaluate the corrections $\delta\phi^{\alpha\beta}$ instead, it is not possible to find a general expression valid at all orders $n$, which therefore have to be considered separately. We choose $t_0$ as an integer multiple of the oscillation period $2\pi/\tilde{\omega}$ (so that the motional state is left unchanged after gate operation), and find

$$\delta\phi^{\alpha\beta} = 3(\alpha-\beta)\sqrt{\frac{\pi}{8}} \xi^2 \epsilon \tilde{\omega}\tau \left[ \frac{1}{\sqrt{2}\xi} \frac{a_{\tilde{\omega}}}{d} + (\alpha-\beta)\left(\frac{a_{\tilde{\omega}}}{d}\right)^2 \right] \times \frac{1}{\hbar\tilde{\omega}} \{E_1 + E_2 + 2\sqrt{E_1 E_2}\cos[\tilde{\omega}(t_1 - t_2)]\} + o((a_{\tilde{\omega}}/d)^3), \quad (4.11)$$

where it has been taken into account that $\omega\tau \gg 1$. The two terms in square brackets in Eq. (4.11) come from terms in the Coulomb potential with $n=3$ and $n=4$ in Eq. (4.2), respectively. This means that no thermal correction is to be expected if only harmonic contributions to the potential (i.e., with $n \leqslant 2$) are included. Indeed, in this case the spurious interaction phases, due to the oscillations in the ions' positions, are averaged out when integrating over a time much larger than the oscillation period. This explains intuitively why the phase does not depend on the motional state, in the

approximation where only linear and quadratic terms in the Coulomb potential are taken into account, as will be shown analytically in Sec. V A. Now, the classical analog of the gate phase Eq. (2.8) can be written as

$$\begin{aligned}\vartheta_{\rm cl} &\equiv \sum_{\alpha,\beta} (-1)^{\alpha+\beta}\varphi_{\rm cl}^{\alpha\beta} \\ &= \sqrt{\frac{\pi}{8}}\frac{\epsilon\omega\tau}{(a_\omega/d)^2}\mathrm{Li}_{1/2}((\xi a_\omega/d)^2) \\ &= \theta_{\rm cl} + o((a_{\tilde\omega}/d)^2),\end{aligned} \tag{4.12}$$

where $\mathrm{Li}_n(z)\equiv\Sigma_{k=1}^{\infty} z^k/k^n$ is the polylogarithm function, and

$$\theta_{\rm cl} \equiv \sqrt{\frac{\pi}{8}}\xi^2\epsilon\tilde\omega\tau. \tag{4.13}$$

From Eqs. (4.12) and (4.13), we see that in our one-dimensional classical model, up to first order in powers of $a_{\tilde\omega}/d$, the gate phase is insensitive to motional excitations inside each trap. Later on (see Sec. V E), we will find that the very same expression for the gate phase can be obtained, under the same approximations, with the full three-dimensional quantum formalism. Moreover, note that assumption (ii) applied to Eq. (4.9) means $\xi\approx 1$, whence (i) implies $\omega\tau\gg 1$. It follows that, if we want to obtain $\theta_{\rm cl}=\pi$, $\epsilon\ll 1$. This means that the confinement has to be strong with respect to Coulomb interaction over the interwell separation, which is in turn consistent with assumption (iii).

We will now consider a more general initial condition than the ones discussed so far, namely, a thermal state, described by a probability distribution over the energies $E_i$ and the oscillation phases $\tilde\omega t_i$. Assuming the energy distribution characteristic of a canonical ensemble and a uniform probability distribution for $\omega t_1$ and $\omega t_2$, we can compute the thermally averaged phase

$$\begin{aligned}\langle\langle\varphi_{\rm cl}^{\alpha\beta}\rangle\rangle &\equiv \int_0^{2\pi/\omega}\frac{dt_1dt_2}{(2\pi/\omega)^2}\int_0^{\infty}\frac{dE_1dE_2}{(k_BT)^2}\varphi_{\rm cl}^{\alpha\beta}e^{-(E_1+E_2)/k_BT} \\ &= -\theta_{\rm cl}\left\{\frac{1}{2}+\frac{\alpha-\beta}{\sqrt{2}\xi}\left[\frac{d}{a_{\tilde\omega}}+\frac{a_{\tilde\omega}}{d}\left(\frac{\xi^2}{\sqrt{3}}+\frac{6k_BT}{\hbar\tilde\omega}\right)\right]\right. \\ &\quad \left.+\left(\frac{a_{\tilde\omega}}{d}\right)^2\left(\frac{\xi^2}{2\sqrt{2}}+\frac{6k_BT}{\hbar\tilde\omega}\right)\right\}\delta_{\alpha\beta}+o((a_{\tilde\omega}/d)^3).\end{aligned} \tag{4.14}$$

The mean gate phase turns out to be

$$\begin{aligned}\langle\langle\vartheta_{\rm cl}\rangle\rangle &\equiv \sum_{\alpha,\beta}(-1)^{\alpha+\beta}\langle\langle\varphi_{\rm cl}^{\alpha\beta}\rangle\rangle \\ &= \theta_{\rm cl}\left[1+\left(\frac{a_{\tilde\omega}}{d}\right)^2\left(\frac{\xi^2}{\sqrt{2}}+\frac{6k_BT}{\hbar\tilde\omega}\right)\right]+o((a_{\tilde\omega}/d)^3),\end{aligned} \tag{4.15}$$

We will see that the very same structure for the corrections to the lowest-order phase is obtained with the full quantum mechanical calculation.

### C. Gate fidelity

In order to obtain the desired phase gate Eq. (2.1), we require that $\langle\langle\vartheta_{\rm cl}\rangle\rangle=\pi$. So the reference state, representing the ideal evolution, is chosen as

$$|\chi'_{\rm cl}\rangle \equiv \sum_{\alpha\beta} c_{\alpha\beta}|\alpha\rangle|\beta\rangle e^{i\langle\langle\varphi_{\rm cl}^{\alpha\beta}\rangle\rangle}. \tag{4.16}$$

The real evolved state, Eq. (4.3), can be written as $|\chi_{\rm cl}(t)\rangle = |\chi'_{\rm cl}\rangle + |\delta\chi_{\rm cl}\rangle$, whereby

$$|\delta\chi_{\rm cl}\rangle \equiv \sum_{\alpha\beta} c_{\alpha\beta}|\alpha\rangle|\beta\rangle(e^{i\varphi_{\rm cl}^{\alpha\beta}}-e^{i\langle\langle\varphi_{\rm cl}^{\alpha\beta}\rangle\rangle}). \tag{4.17}$$

In our classical model, we are treating our particles' external degrees of freedom classically. Therefore, in the evaluation of the fidelity Eq. (2.5), instead of tracing over the motional eigenstates we should average over the possible classical trajectories. Thus

$$\begin{aligned}F_{\rm cl} &\equiv \min_{\chi}\langle\langle\langle\chi'_{\rm cl}|\chi_{\rm cl}(t)\rangle\langle\chi_{\rm cl}(t)|\chi'_{\rm cl}\rangle\rangle\rangle \\ &= \min_{\chi}\langle\langle|1+\langle\chi_{\rm cl}(t)|\delta\chi_{\rm cl}\rangle|^2\rangle\rangle \\ &\overset{(4.17)}{=} \min_{\{c_{\alpha\beta}\}}\left\langle\left\langle\left|\sum_{\alpha,\beta=0}^{1}|c_{\alpha\beta}|^2e^{-i(\varphi_{\rm cl}^{\alpha\beta}-\langle\langle\varphi_{\rm cl}^{\alpha\beta}\rangle\rangle)}\right|^2\right\rangle\right\rangle = 1 \\ &\quad -\left(\frac{6\theta_{\rm cl}k_BT}{\hbar\tilde\omega}\right)^2\left[\frac{1}{\xi^2}\left(\frac{a_{\tilde\omega}}{d}\right)^2-2\left(\frac{a_{\tilde\omega}}{d}\right)^4\right]+o((a_{\tilde\omega}/d)^5),\end{aligned} \tag{4.18}$$

as discussed in detail in Appendix A 2. Finally, let us consider what would come out if we were able to suppress the cubic anharmonic correction from the Coulomb potential, i.e., to put $\kappa=0$. We will show later (Sec. V D) how this can be done in practice—here we would like to give a classical estimate $F'_{\rm cl}$ of the improved gate fidelity. The calculation is performed in Appendix A 2 as well, and the result is

$$F'_{\rm cl}(T) = 1-\left(\frac{3\theta_{\rm cl}k_BT}{\hbar\tilde\omega}\right)^2\left(\frac{a_{\tilde\omega}}{d}\right)^4+o((a_{\tilde\omega}/d)^5). \tag{4.19}$$

This shows that, by suppressing one order of anharmonic corrections, one obtains an improvement by two orders in $a_\omega/d$ (several orders of magnitude) in the fidelity, as is shown in Fig. 3.

## V. QUANTUM TREATMENT

We want to describe quantum mechanically the three-dimensional dynamics of the two particles. This means that, unlike in the previous section, their motional state is given

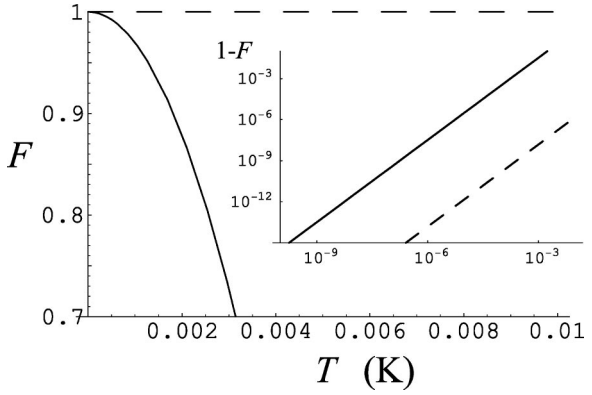


FIG. 3. Fidelity $F_{\mathrm{cl}}$ (solid line) and improved fidelity $F'_{\mathrm{cl}}$ (dashed line) in the classical model as a function of temperature $T$. Inset: detail of the departure from unity of the same quantities, on a logarithmic scale. We assumed use of $Ca^{+}$ ions and chose the parameters $\omega = 2\pi \times 1$ MHz, $d = 20$ $\mu$m.

by a wave function (see Fig. 4) which evolves according to the Hamiltonian Eq. (2.4). To better understand its structure, it is useful to write

$$H^{\alpha\beta}(t,\hat{\mathbf{x}}_1,\hat{\mathbf{x}}_2) \equiv H^{\alpha\beta}(t,\mathbf{x}^{\alpha}(t),\mathbf{x}^{\beta}(t)) + H_e^{\alpha\beta}(t,\hat{\mathbf{x}}_1,\hat{\mathbf{x}}_2). \tag{5.1}$$

Here the $\hat{\mathbf{x}}_j$ are the ion position operators, and the $c$ numbers $\mathbf{x}^{\alpha_j}(t)$ denote the centers of the initial motional wave functions as determined by the trap (see Sec. III). To second order in the expansion Eq. (4.2), the first term on the right-hand side of Eq. (5.1) gives rise to the same contribution to the phase already calculated in lowest order in the classical model, namely, $\theta_{\mathrm{cl}}$ given in Eq. (4.13). Corrections to this phase are due, as before, to (a) thermal excitations; (b) higher-order (multipole) terms in the expansion of the Coulomb potential; (c) nonadiabaticity. Motional effects of the kinds (a) and (c) are accounted for by $H_e^{\alpha\beta}$, while multipole corrections get a contribution also from $H^{\alpha\beta}(t,\mathbf{x}^{\alpha}(t),\mathbf{x}^{\beta}(t))$. In order to minimize such corrections, we choose to operate in the adiabatic regime, given by condition (i) in Sec. IV, i.e., we assume $\omega\tau \gg 1$. We study the dynamics in the center-of-mass and relative coordinate systems, as given by Eqs. (3.5a) and (3.5b). In both coordinate systems, the motion along different axes decouples: the transverse directions contribute just an overall phase, whereas the relevant state-dependent dynamics takes place along the $x$ axis. Since we assumed $d \gg a_\omega$, it follows that $H_1$—containing only terms of $o((a_\omega/d)^3)$—can be treated as a small perturbation in $H$. We will first neglect it and solve exactly the three-dimensional Schrödinger equation, and then take it into account perturbatively, eventually checking our results with a numerical simulation.

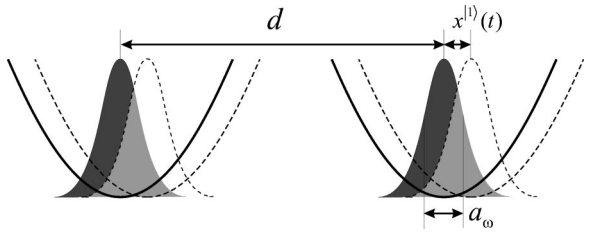


FIG. 4. Gate operation scheme in the quantum regime. Trap parameters are defined as in the classical case; the harmonic oscillator ground-state width $a_\omega$ is also shown.

### A. Unperturbed forced oscillator

When we put $H_1 = 0$ and take $\mathcal{F}(t)$ as in Eq. (4.9), the solution to Eq. (B4) can be written explicitly [10]. This is done in Appendix B 2. The gate phase turns out to be, in this approximation,

$$\theta \equiv \sum_{\alpha,\beta} (-1)^{\alpha+\beta} \phi^{\alpha\beta} = 2\xi^2 [\Phi(\omega) - \Phi(\omega\sqrt{1+\epsilon})], \tag{5.2}$$

where

$$\Phi(\omega) \equiv -\mathrm{Im}\left[ \int_{t_0}^{t} ds K(s,t_0) \frac{dK^*(s,t_0)}{ds} \right], \tag{5.3a}$$

$$K(t,t_0) \equiv \frac{1}{\sqrt{m\hbar\omega}} \int_{t_0}^{t} dt' \mathcal{F}(t') e^{i\omega(t'-t_0)}. \tag{5.3b}$$

Explicit expressions for $\phi^{\alpha\beta}$ and for $\Phi(\omega)$ are given in Eqs. (B12a)–(B12d). In the limit $\omega\tau \gg 1$, we obtain $\Phi(\omega) \approx -\sqrt{\pi/32}\,\omega\tau$. By expanding Eq. (5.2) up to first order in $\epsilon$, we retrieve $\theta \approx \theta_{\mathrm{cl}}$ as given by Eq. (4.13). The phase $\theta$ can be adjusted to the desired value $\pi$ by tuning the displacement $\xi$ and/or the interaction time $\tau$. Moreover, $\theta$ is independent of the ions' motional state. This means that the phase remains the same even if we start with a mixed external state, described by a density matrix

$$\rho_T(t_0) \equiv \frac{e^{-H(t_0)/k_B T}}{Z} \approx (1-\gamma)^6 \bigotimes_{i=1}^{6} \sum_{n_i=1}^{\infty} \gamma^{n_i} |n_i\rangle_i \langle n_i|, \tag{5.4}$$

corresponding to a thermal distribution at temperature $T$. Here the canonical partition function $Z \equiv \mathrm{tr}\{e^{-H(t_0)/k_B T}\}$, $\gamma \equiv \exp(-\hbar\omega/k_B T)$, $\{n_i\}_{i=1,\cdots,6} \equiv \{n_x, n_y, n_z, N_X, N_Y, N_Z\}$, and the $|N\rangle_{X,Y,Z}$ ($|n\rangle_{x,y,z}$) are the eigenstates of $H_R^0$ ($H_r^0$) along each direction. To optimize the gate fidelity (see Sec. II), we need one thing more—that the external degrees of freedom are not entangled with the internal ones after gate operation, i.e., that the final motional state does not depend on the logical states of the qubits. This indeed happens, under the adiabatic assumption (i) of Sec. IV. In fact, in this case, the overlap $\mathcal{O}^{\{n_i\}}(t,t_0)$ between the initial and final spatial wavefunctions for a system starting in a motional eigenstate along all degrees of freedom, defined by Eq. (B14), is close to 1. To be more precise, $\mathcal{O}^{\{n_i\}}(t,t_0)$ formally depends on the motional state; however, if the adiabatic condition is satisfied and $|t|, |t_0|$ are large enough, $\mathcal{O}^{\{n_i\}}(t,t_0)$ tends exponentially to 1, as can be seen from Eqs. (B15a) and (B15b).

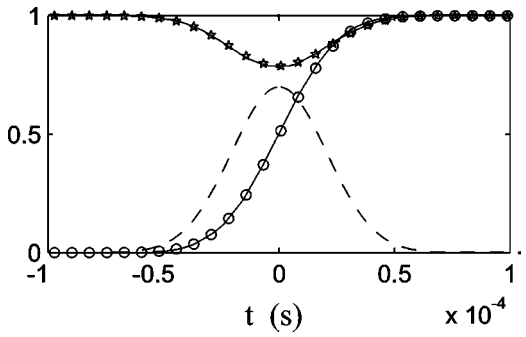


FIG. 5. Gate phase $\vartheta/\pi$ (circles), and projection of the initial motional ground state over the evolved one for ions in states $|0\rangle_1|1\rangle_2$ (stars), as induced by the external force $\mathcal{F}(t)$ (dashed line). The results of the numerical calculation, performed with the parameters quoted in the text including corrections up to $o((a_\omega)^5)$, are shown. Solid lines are analytical results in the harmonic approximation of Sec. V A.

### B. Including higher-order terms

We will now take into account the contribution of $H_1$. This does not affect the center-of-mass motion. Therefore from now on we will study only the relative motion. A little care is needed since, unlike in the most common time-dependent perturbation theory, in our case the unperturbed Hamiltonian depends on time, while the perturbation does not. The calculation is carried out in Appendix B 3. In the adiabatic limit and for $|t|,|t_0|>\tau$, first-order corrections simply amount to a relatively small additional phase shift:

$$\langle U(t,t_0)\rangle \approx \langle U_0(t,t_0)\rangle e^{i(\Delta^{\alpha\beta}+\Delta')}. \tag{5.5}$$

Thus, to this order,

$$\varphi^{\alpha\beta} \approx \phi^{\alpha\beta}+\Delta^{\alpha\beta}+\Delta'. \tag{5.6}$$

Hence we find $\vartheta=\theta+\delta\theta+o[(a_\omega/d)^6]$, where

$$\delta\theta = 8\frac{a_\omega^2}{d^2}\theta_{\rm cl}[\sqrt{2}\xi^2+3(2n_x-n_y-n_z)], \tag{5.7}$$

and it is understood that we started from a pure state with $n_{x,y,z}$ excitations along the various directions of the relative motion. As already anticipated, Eq. (5.7) has the same structure as the classical correction to the phase expressed by Eq. (4.15), except for a different overall factor related to the dimensionality of the problem we are now considering. Indeed, the first term in square brackets comes from the higher multipoles ($k=3$) in $H_1$, while the second one is due to the thermal excitations.

### C. Numerical computation

In order to check the validity of the perturbative expression Eq. (5.7), we solved the Schrödinger equation for the relative motion numerically, taking into account cubic and quartic interaction terms, explicitly given by Eqs. (A6a) and (A6b) respectively. The calculation is described in Appendix B 5, and results are shown in Fig. 5. In particular we find that the cubic corrections cancel each other, and that the quartic corrections have the same order of magnitude as predicted by Eq. (5.7). From Eq. (5.2) we obtain $\theta=\pi$ with $\omega=2\pi\times 1$ MHz, $\overline{x_2}-\overline{x_1}=20$ $\mu$m, $\xi=0.7$, and $\tau=41.1069$ $\mu$s. These results were confirmed by a numerical computation including up to 40 initial excitations in each direction, always giving unity overlap of the final motional state with the initial one. Indeed, with $t=-t_0=150$ $\mu$s, even starting, e.g., with the $(10^4)$th oscillator excited state, Eq. (B14) still predicts $\mathcal{O}(t,t_0)>1-10^{-10}$. With these parameters, the perturbative estimate derived within the classical model in Sec. IV turns out to be $\theta_{\rm cl}\approx 1.04\pi$.

### D. Gate fidelity

The gate phase $\vartheta$ cannot be measured directly, since the higher-order corrections arising from the Coulomb potential depend both on the internal and on the motional state of each ion, and cannot be undone by means of single-qubit operations, unless the logical state is measured. However, the corrections of order $k$ have a simple internal-state dependence of the kind $(\alpha-\beta)^k$, as shown by Eq. (B22a). This implies that it is possible to obtain a cancellation of the odd-order corrections, by applying a $\pi$ pulse $R\equiv|0\rangle\langle 1|+|1\rangle\langle 0|$ to both qubits in the middle of gate operation. Indeed, if $U$ is the evolution operator giving the dynamics described in the previous sections, we find

$$\begin{aligned}
&|0\rangle|0\rangle \overset{RU}{\rightarrow} e^{i\varphi^{00}}|1\rangle|1\rangle \overset{RU}{\rightarrow} e^{i(\varphi^{00}+\varphi^{11})}|0\rangle|0\rangle,\\
&|0\rangle|1\rangle \rightarrow e^{i\varphi^{01}}|1\rangle|0\rangle \rightarrow e^{i(\varphi^{01}+\varphi^{10})}|0\rangle|1\rangle,\\
&|1\rangle|0\rangle \rightarrow e^{i\varphi^{10}}|0\rangle|1\rangle \rightarrow e^{i(\varphi^{10}+\varphi^{01})}|1\rangle|0\rangle,\\
&|1\rangle|1\rangle \rightarrow e^{i\varphi^{11}}|0\rangle|0\rangle \rightarrow e^{i(\varphi^{11}+\varphi^{00})}|1\rangle|1\rangle.
\end{aligned} \tag{5.8}$$

Here an adiabatic approximation is understood, according to which the final and initial motional states are identical. We now define

$$\Delta\theta \equiv \delta\theta - \langle\langle \delta\theta\rangle\rangle \tag{5.9}$$

(as before, $\langle\langle\cdot\rangle\rangle$ denotes the thermal average), and the gate operator

$$G \equiv S(RU)^2, \tag{5.10}$$

where

$$S \equiv |0\rangle\langle 0|e^{-2i\xi^2\Phi(\omega)}+|1\rangle\langle 1|e^{-i[2\xi^2\Phi(\omega\sqrt{1+\epsilon})-\langle\langle\delta\theta\rangle\rangle]}. \tag{5.11}$$

If we choose the gate operation time $\tau$ in such a way that

$$\pi \overset{!}{=} 4\xi^2[\Phi(\omega)-\Phi(\omega\sqrt{1+\epsilon})]-2\langle\langle\delta\theta\rangle\rangle, \tag{5.12}$$

we obtain

$$
\begin{aligned}
|0\rangle|0\rangle &\overset{G}{\rightarrow} e^{i\Theta}|0\rangle|0\rangle,\\
|0\rangle|1\rangle &\rightarrow e^{-i\Delta\theta}e^{i\Theta}|0\rangle|1\rangle,\\
|1\rangle|0\rangle &\rightarrow e^{-i\Delta\theta}e^{i\Theta}|1\rangle|0\rangle,\\
|1\rangle|1\rangle &\rightarrow e^{i\pi}e^{i\Theta}|1\rangle|1\rangle.
\end{aligned}
\tag{5.13}
$$

The global (thus irrelevant) phase $\Theta$ is given in Appendix B 6. Note that the single-qubit rotation $S$ is the same for both qubits, and therefore single-ion addressability is not required. The fidelity of the gate operation is defined by comparing the ideal gate operation Eq. (2.1) with the actual dynamics obtained in our scheme, Eq. (5.13), at a given temperature $T$ for the motion in all three dimensions. The result, derived in Appendix B 6, is

$$
F(T)\approx 1-6^3\left(\frac{\theta_{\rm cl}k_BT}{\hbar\omega}\right)^2\left(\frac{a_\omega}{d}\right)^4. \tag{5.14}
$$

The fidelity turns out to be independent of $\tau$ and $\xi$ which, subject to the conditions $\omega\tau\gg 1$ and $\xi\sim 1$, can be freely chosen to obtain the desired gate phase. The dependence of the fidelity on the various parameters is the same as in the classical model discussed in the previous section. As already anticipated in the previous section, the intermediate $\pi$ pulse $R$ allows us to get rid of the $o((a_\omega/d)^2)$ term, thus obtaining a much better gate performance. Indeed, the only difference between the corrected classical fidelity $F'_{\rm cl}$ and the quantum fidelity $F$ is the numerical prefactor multiplying the temperature-dependent part, which is bigger in the latter case due to the inclusion of all the spatial degrees of freedom, whereas our classical model was just one dimensional. Anyway, with the parameters quoted above, at temperatures below 2 mK, corresponding to an average number of harmonic oscillator excitations $\overline{n}\sim 6$, the fidelity turns out to be bigger than $1-10^{-6}$. We can also evaluate how the fidelity scales when the gate is repeatedly applied, say $g$ times. It is clear from Eq. (5.13) that in this case, apart again from an overall phase,

$$
\begin{aligned}
|0\rangle|0\rangle &\overset{G_g}{\rightarrow} |0\rangle|0\rangle,\\
|0\rangle|1\rangle &\rightarrow e^{-ig\Delta\theta}|0\rangle|1\rangle,\\
|1\rangle|0\rangle &\rightarrow e^{-ig\Delta\theta}|1\rangle|0\rangle,\\
|1\rangle|1\rangle &\rightarrow (-1)^g|1\rangle|1\rangle.
\end{aligned}
\tag{5.15}
$$

The excitation-dependent phase $\Delta\theta$ is just multiplied by $g$. Thus, under the same approximations as above, the fidelity of the $g$-fold gate operation is

$$
F^{(g)}(T)=1-g^2[1-F(T)], \tag{5.16}
$$

i.e., it scales with the square of the number of gates.

### E. One-dimensional calculation for many ions

We now assume we have $N$ ions, trapped in a linear array of equally spaced traps, i.e., we take

$$
\overline{\mathbf{r}}_j\equiv(\overline{x}_j,\overline{y}_j,\overline{z}_j)=j\mathbf{d} \tag{5.17}
$$

in Eq. (3.2a). Expanding the interaction Hamiltonian $H_{ij}$, Eq. (3.2b), in powers of the $\mathbf{r}_i$ and $\mathbf{r}_j$, and neglecting terms of $o((a_\omega/d)^3)$, we find

$$
\begin{aligned}
H\approx\frac{m\omega^2}{2}\Bigg\{\sum_{i=1}^N\Bigg[&\frac{\omega_i^2}{\omega^2}(x_i-\tilde{x}_i)^2+y_i^2+z_i^2-\varepsilon_i\\
&-2a_\omega\mathcal{F}(t)|1\rangle_i\langle 1|(x_i+\overline{x}_i)\Bigg]+\epsilon\sum_{i<j}^N\frac{x_ix_j}{|i-j|^3}\Bigg\},
\end{aligned}
\tag{5.18}
$$

where the various quantities are defined in Appendix B 7. Equation (5.18) describes a set of independent forced harmonic oscillators, like the ones we solve in Appendix B 2, plus a coupling term multiplied by $\epsilon$. If $\epsilon\ll 1$, we can treat this term as a small perturbation, in the very same way we develop in Appendix B 3. We take as initial state

$$
|\Psi_N(t_0)\rangle=\prod_{i=1}^N|\mathbf{n}_i\rangle_i|\alpha_i\rangle_i, \tag{5.19}
$$

where $\alpha_i$ denotes the internal state of the $i$th ion and $\mathbf{n}_i$ its motional state in the well corresponding to the $i$th term of the first sum on the right-hand side of Eq. (5.18). We obtain

$$
|\Psi_N(t)\rangle\approx\frac{1}{2}\prod_{i=1}^N\left(e^{i\phi^{\alpha_i}}\prod_{j\neq i}e^{i\phi^{\alpha_i\alpha_j}}\right)|\Psi_N(t_0)\rangle, \tag{5.20}
$$

where (calculating the two-particle phases $\phi^{\alpha_i\alpha_j}$ perturbatively)

$$
\begin{aligned}
\phi^{\alpha_i}\approx&\,\alpha_i^2\xi^2\Phi(\omega_i)+\alpha_i\sqrt{\pi}\omega\tau\xi\overline{x}_i/a_\omega\\
&-[n_{x,i}\omega_i+(n_{y,i}+n_{z,i})\omega](t-t_0),
\end{aligned}
\tag{5.21a}
$$

$$
\begin{aligned}
\phi^{\alpha_i\alpha_j}&\approx\epsilon\int_{t_0}^t\langle\Psi_N(t_0)|U_0(t,t')\frac{x_ix_j}{|i-j|^3}U_0(t',t_0)|\Psi_N(t_0)\rangle dt'\\
&=\sqrt{\frac{\pi}{8}}\frac{\alpha_i\alpha_j}{|i-j|^3}\frac{\xi^2\epsilon\omega\tau}{(1+\epsilon\eta_i)(1+\epsilon\eta_j)}\approx\frac{\alpha_i\alpha_j}{|i-j|^3}\theta_{\rm cl},
\end{aligned}
\tag{5.21b}
$$

the last line following from $\epsilon\ll 1$ and Eq. (B40). Again, the result to this order turns out to be independent of the motional state of any one of the ions. In the case of two ions, Eq. (5.21b) gives back Eq. (4.13).

## VI. CONCLUSIONS

We analyzed in detail a recent proposal [7] for scalable quantum computation with ions in an array of microtraps.

This scheme has important advantages over the previous proposal [9], based on trapped ions as well. In that case many ions, lying in a single trap minimum, exchange information via collective motional excitations; ground-state cooling is an absolute need, and any perturbation on each ion can affect the performance of the whole system. Here, instead, each ion is confined to a single minimum of a periodic microscopic potential, and interacts with other ions via the Coulomb force. Under the conditions discussed in the text (adiabaticity of the trap displacement, strong confinement with respect to the distance between ions, intermediate symmetrizing $\pi$ pulse), the phase shift is insensitive, to a high accuracy, to the motional state of each ion inside each trap, and therefore the fidelity turns out to be essentially independent of temperature. Moreover, trapping frequencies can be much higher than in the previous case, leading to much shorter gate operation times. As long as we take into account purely motional decoherence mechanisms, we find a fidelity bigger than $1-10^{-6}$ for a two-qubit phase gate operating on a time scale of a few tens of microseconds. Furthermore, with the improved scheme presented here, single-qubit addressability is not required for any of the various control operations. To sum up, the present proposal constitutes a really good candidate for a scalable implementation of a quantum computer.

## ACKNOWLEDGMENTS

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## APPENDIX A: CLASSICAL CALCULATION

In this appendix we give a detailed account of the calculations leading to the results obtained in the classical model for our two-qubit phase gate.

### 1. Rewriting the Hamiltonian

In this section we give the explicit form of the various terms in Eqs. (3.5a) and (3.5b), describing the Hamiltonian Eq. (3.1) for two ions, in the center-of-mass and relative motion coordinate systems. The Hamiltonian, with the number of ions $N=2$, may be rewritten as $H=H_R+H_r$, where

$$H_R=\frac{\mathbf{P}^2}{2M}+\frac{1}{2}M\omega^2\mathbf{R}^2-\mathbf{F}(t)\cdot(\mathbf{R}+\mathbf{R}_0), \tag{A1a}$$

$$H_r=\frac{\mathbf{p}^2}{2\mu}+\frac{1}{2}\mu\omega^2(\mathbf{r}+\mathbf{d}-\mathbf{d}_0)^2-\mathbf{f}(t)\cdot(\mathbf{r}+\mathbf{d})+\frac{\lambda}{|\mathbf{r}+\mathbf{d}|}, \tag{A1b}$$

and

$$\mathbf{R}\equiv(X,Y,Z)\equiv\frac{\mathbf{r}_1+\mathbf{r}_2}{2}-\mathbf{R}_0, \tag{A2a}$$

$$\mathbf{r}\equiv(x,y,z)\equiv\mathbf{r}_2-\mathbf{r}_1-\mathbf{d}, \tag{A2b}$$

$$\mathbf{R}_0\equiv\frac{\overline{\mathbf{r}_1}+\overline{\mathbf{r}_2}}{2},\quad \mathbf{d}_0\equiv|\overline{\mathbf{r}_2}-\overline{\mathbf{r}_1}|=(d_0,0,0), \tag{A2c}$$

$$\mathbf{P}\equiv\mathbf{p}_1+\mathbf{p}_2,\quad \mathbf{p}\equiv\frac{\mathbf{p}_2-\mathbf{p}_1}{2}, \tag{A2d}$$

$$\mathbf{F}(t)\equiv\mathbf{F}_1(t)+\mathbf{F}_2(t),\quad \mathbf{f}(t)\equiv\frac{\mathbf{F}_2(t)-\mathbf{F}_1(t)}{2}, \tag{A2e}$$

$$Mx\equiv 2m,\quad \mu\equiv\frac{m}{2},\quad \lambda\equiv\frac{q_e^2}{4\pi\varepsilon_0}. \tag{A2f}$$

In the above, $\mathbf{d}\equiv(d,0,0)$ is the equilibrium separation between the two particles in the absence of the pushing force. Due to the repulsive Coulomb interaction, $|\mathbf{d}|\equiv d$ will be bigger than the distance $d_0$ between the centers of the two bare harmonic traps, defined in Eq. (A2c). The correction $\delta x\equiv d-d_0$ is the solution of the equation

$$0=\frac{\partial}{\partial x}\left(\frac{1}{2}\mu\omega^2x^2+\frac{\lambda}{|x+d_0|}\right)=\mu\omega^2x-\frac{\lambda}{(x+d_0)^2} \tag{A3}$$

(assuming $d_0+x>0$), and can be written as

$$\delta x=\frac{4d_0}{3}\sinh^2\left\{\frac{1}{6}\ln[\,\eta+1+\sqrt{\eta(\eta+2)}]\right\} \tag{A4}$$

with $\eta\equiv\lambda/[2\mu\omega^2(d_0/3)^3]$. Expanding to first order in $\epsilon$, we find $\delta x\approx\epsilon d_0/2$. Taking into account that, if the traps are sufficiently far apart, the relevant coordinate range is $x_2>x_1$, one obtains the multipole expansion

$$\frac{\lambda}{|\mathbf{r}+\mathbf{d}|}\approx\frac{\lambda}{d}\left[1-\frac{x}{d}+\frac{x^2}{d^2}-\frac{1}{2}\frac{y^2}{d^2}-\frac{1}{2}\frac{z^2}{d^2}+\sum_{k=3}^{\infty}\frac{P_k(x,y,z)}{d^k}\right], \tag{A5}$$

where each of the multipole terms $P_k$ is a polynomial of $k$th degree in $x$, $y$, and $z$; for instance,

$$P_3(x,y,z)=-x\left[x^2-\frac{3}{2}(y^2+z^2)\right], \tag{A6a}$$

$$P_4(x,y,z)=x^4-3x^2(y^2+z^2)+\frac{3}{8}(y^2+z^2)^2. \tag{A6b}$$

By virtue of Eq. (A3), the linear term in the expansion Eq. (A5) cancels exactly with the one arising from the harmonic potential $\mu\omega^2(\mathbf{r}+\mathbf{d}-\mathbf{d}_0)^2/2$ in Eq. (A1b). We define the unperturbed Hamiltonians

$$H_R^0\equiv\frac{\mathbf{P}^2}{2M}+\frac{1}{2}M\omega^2\mathbf{R}^2,\quad H_r^0\equiv H_x+H_\perp, \tag{A7}$$

where

$$H_x\equiv\frac{p_x^2}{2\mu}+\frac{1}{2}\mu\nu^2x^2, \tag{A8a}$$

$$H_{\perp} \equiv \frac{p_y^2+p_z^2}{2\mu} + \frac{1}{2}\mu\nu_{\perp}^2(y^2+z^2); \tag{A8b}$$

the higher-multipole contribution

$$H_1 \equiv \frac{\lambda}{d}\sum_{k=3}^{\infty}\frac{P_k(x,y,z)}{d^k}; \tag{A9}$$

the force terms

$$F(t) = \frac{\hbar\omega}{a_\omega}(\hat{\Pi}_1+\hat{\Pi}_2)\mathcal{F}(t), \quad f(t) = \frac{\hbar\omega}{a_\omega}\frac{\hat{\Pi}_2-\hat{\Pi}_1}{2}\mathcal{F}(t), \tag{A10}$$

where $\hat{\Pi}_i^{\alpha}$ is the projector onto the internal state $\alpha$ of particle $i$,

$$\hat{\Pi}_1 \equiv |1\rangle_1\langle 1|\otimes \mathbf{1}_2, \quad \hat{\Pi}_2 \equiv \mathbf{1}_1\otimes|1\rangle_2\langle 1|; \tag{A11}$$

the rescaled frequencies

$$\nu \equiv \omega\sqrt{1+\epsilon}, \quad \nu_{\perp} \equiv \omega\sqrt{1-\epsilon/2}; \tag{A12}$$

and the shifted coordinate and energy scales

$$X_0 \equiv \mathbf{R}_0\cdot(1,0,0), \quad E_0 \equiv \frac{\lambda}{d}+\frac{1}{2}\mu\omega^2\delta x^2. \tag{A13}$$

Shifting the coordinate system by $\mathbf{R}_0-\mathbf{d}$ and the energy scale by $E_0$, we finally obtain Eqs. (3.5a) and (3.5b).

### 2. Fidelity

The goal of this section is to show the derivation of the analytical temperature dependence of the fidelity, Eq. (4.19). We begin by writing the two-particle phase as

$$\varphi_{\rm cl}^{\alpha\beta} - \langle\langle\varphi_{\rm cl}^{\alpha\beta}\rangle\rangle = \delta_{\alpha\beta}[(-1)^{\beta}\kappa+1]\varepsilon + o((a_{\tilde{\omega}}/d)^3), \tag{A14}$$

where

$$\kappa \equiv \frac{d}{\sqrt{2}\xi a_{\tilde{\omega}}}, \tag{A15a}$$

$$\varepsilon = \frac{3\theta_{\rm cl}}{\hbar\tilde{\omega}}\left(\frac{a_{\tilde{\omega}}}{d}\right)^2\{E_1+E_2-2\sqrt{E_1E_2}\cos[\tilde{\omega}(t_1-t_2)]-2k_BT\}. \tag{A15b}$$

We define

$$\begin{aligned}\Xi(a,b) &\equiv |\langle\chi'_{\rm cl}|\chi_{\rm cl}(t)\rangle|^2 \\ &= 2(a\{1-\cos[(\kappa-1)\varepsilon]\}-b\cos[(\kappa-1)\varepsilon]) \\ &\quad\times(a+b-1)+(b-1)^2+b[b+2a\cos(2\kappa\varepsilon)],\end{aligned} \tag{A16}$$

where $a \equiv |c_{01}|^2$, $b \equiv |c_{10}|^2$, and the normalization of $|\chi_{\rm cl}\rangle$, in the form $1=\Sigma_{\alpha,\beta}|c_{\alpha\beta}|^2$, has been taken into account. From Eq. (4.18) it follows that

$$F_{\rm cl} = \min_{\{a,b\}}\langle\langle\Xi(a,b)\rangle\rangle = \langle\langle\min_{\{a,b}\}\Xi(a,b)\rangle\rangle, \tag{A17}$$

which is a constrained minimization problem, with constraints $0\leqslant a\leqslant 1$, $0\leqslant b\leqslant 1$. The solution cannot be found by simply equating the partial derivatives of $\Xi(a,b)$ to zero, since—as will be seen at the end of this section—the minimum turns out to be located at the border of the region of allowed parameters. Therefore we must take a closer look at the problem to find the analytical solution. To this end, we evaluate

$$\partial_a\Xi(a,b) = -2\varepsilon^2(\kappa-1)^2\left(b\frac{\kappa+1}{\kappa-1}+\frac{1}{2}-a\right)+o(\varepsilon^4), \tag{A18a}$$

$$\partial_b\Xi(a,b) = -2\varepsilon^2(\kappa+1)^2\left(a\frac{\kappa-1}{\kappa+1}+\frac{1}{2}-b\right)+o(\varepsilon^4). \tag{A18b}$$

While looking for the minimum, we will neglect $o(\varepsilon^4)$ $\propto(a_\omega/d)^8$; then, to evaluate it, we will use the exact form of $\Xi(a,b)$. According to Eq. (A18a), in the region of the parameter plane defined by the condition

$$b \leqslant \left(a-\frac{1}{2}\right)\frac{\kappa-1}{\kappa+1}, \tag{A19}$$

$\partial_b\Xi(a,b)\leqslant -2\kappa(\kappa+1)<0$. Since $\kappa>1$, the inequality Eq. (A19) also implies $b<1/2$. Therefore the minimum must be found outside the region defined by Eq. (A19), i.e., for

$$a < b\frac{\kappa+1}{\kappa-1}+\frac{1}{2}. \tag{A20}$$

The latter, by Eq. (A18b), implies $\partial_a\Xi(a,b)<0$. Summing up, the minimum is reached for the values $(a_0,b_0)$ of the parameters, where

$$a_0 = 1, \quad \frac{1}{2}\frac{\kappa-1}{\kappa+1} < b_0 \leqslant 1. \tag{A21}$$

The problem is therefore reduced to a one-dimensional constrained minimization: We have to study the equation

$$\begin{aligned}0 &= \partial_b\Xi(a_0,b) \\ &= 2(\cos(2\kappa\varepsilon)-\cos[(\kappa-1)\varepsilon]-2b\{\cos[(\kappa+1)\varepsilon]-1\}),\end{aligned} \tag{A22}$$

which has the solution

$$\bar{b} \equiv \frac{1}{2}\frac{\sin[(3\kappa-1)\varepsilon/2]}{\sin[(\kappa+1)\varepsilon/2]}. \tag{A23}$$

Since the constraint $b_0\leqslant 1$ has to be fulfilled, we obtain $b_0 = \min\{\bar{b},1\}$. Indeed, it is $\bar{b}\leqslant 1$ only for $\varepsilon\geqslant f_\kappa(\varepsilon)$, where

$$f_\kappa(\varepsilon)\equiv 2\arcsin\left[\frac{\sin(3\kappa\varepsilon/2)-2\sin(\kappa\varepsilon)}{\sqrt{5+4\cos(2\kappa\varepsilon)}}\right]. \quad \text{(A24)}$$

Hence, to $o((a_\omega/d)^4)$,

$$F_{\rm cl}\approx\begin{cases}\frac{1}{2}\{1+\langle\langle\cos[(3\kappa-1)\varepsilon]\rangle\rangle\}, & \varepsilon\geqslant f_\kappa(\varepsilon)\\ 1-4\langle\langle\cos(\kappa\varepsilon)[\cos(\varepsilon)-\cos(\kappa\varepsilon)]\rangle\rangle & \text{otherwise.}\end{cases} \quad \text{(A25)}$$

Now, $f'_\kappa(0)=\kappa/3>1$ (the inequality following from $a_\omega \ll d$). Hence for small $T$—such that $\langle\langle\varepsilon\rangle\rangle\ll 1$, i.e., $k_BT \ll \hbar\omega(d/a_\omega)^2$—we have $\varepsilon<f_\kappa(\varepsilon)$ and the form of $F_{\rm cl}$ is given by the second row on the right-hand side of Eq. (A25), which we can expand in a Taylor series around $T=0$, taking the thermal average to finally obtain Eq. (4.18). When $\kappa=0$, i.e., the third-order anharmonic correction is suppressed,

$$\Xi(a,b)|_{\kappa=0}=1+2(a+b-1)(a+b)[1-\cos(\varepsilon)]. \quad \text{(A26)}$$

The function to be minimized depends now only on the sum $a+b$. Therefore the minimum can be searched for by fixing one of the two parameters and varying only the other one. We can choose $a_0=1$ as before, and minimize Eq. (A26) with respect to $b$. Equation (A25) gives the solution in this case also. In particular, since $f_{\kappa=0}(\varepsilon)\equiv 0<\varepsilon\,\forall\varepsilon$, the analytical expression for the fidelity is now given by the first row on the right-hand side of Eq. (A25), which for $\kappa=0$ becomes simply

$$F'_{\rm cl}\equiv F_{\rm cl}|_{\kappa=0}\approx\frac{1}{2}[1+\langle\langle\cos(\varepsilon)\rangle\rangle]. \quad \text{(A27)}$$

The same procedure can also be used for the minimization over the possible internal states in the quantum case, as is done in Appendix B 6. By expanding Eq. (A27) to lowest nonzero order in powers of $a_\omega/d$, we finally obtain Eq. (4.19).

## APPENDIX B: QUANTUM CALCULATION

In this appendix we compute both analytically and numerically the evolution of the two-ion system, evaluate the resulting phase shifts, and derive an accurate expression for the fidelity, giving also the explicit expression of some quantities used in the text.

### 1. Undoing single-particle phases

In this section we show how to get rid of the spurious phases accumulated during gate operation, in order to be left with the gate phase Eq. (2.8). In the ideal case where the external degrees of freedom factorize out at the end of the computation, the evolution operator Eq. (2.7) induces both two-particle conditional phases and single-particle kinetic phases, depending on each ion's external state. When both particles are in their external ground state, we can undo the kinetic phases and other inessential phases through single-bit operations of the form

$$S_j=e^{-i\varphi_j}\sum_\alpha |\alpha\rangle_j\langle\alpha|e^{is_j^\alpha}, \quad \text{(B1)}$$

where $\varphi_j$ has to be equal to the kinetic phase acquired after the gate operation by particle $j$, and we choose

$$s_1^0=-\varphi^{00}/2,\quad s_1^1=-\varphi^{10}+s_1^0;\qquad s_2^0=s_1^0,\quad s_2^1=-\varphi^{01}+s_1^0. \quad \text{(B2)}$$

Under these conditions, the compound operator

$$\mathcal{U}(t)\equiv(S_1\otimes S_2)U(t,t_0) \quad \text{(B3)}$$

implements the transformation Eq. (2.1), with $\vartheta$ given by Eq. (2.8).

### 2. Unperturbed solution

As explained in the text, since we assume $d\gg a_\omega$ we can treat the higher-multipole term $H_1$ as a small perturbation with respect to the rest of the Hamiltonian. In this section we solve the unperturbed problem exactly, i.e., we calculate the time-dependent evolution dictated by $H(t)-H_1$. So we want to solve the Schrödinger equation

$$i\hbar|\dot\Psi(t)\rangle=[H_R(t)+H_r^0(t)-\mathbf{f}(t)\cdot(\mathbf{r}+\mathbf{d})]|\Psi(t)\rangle, \quad \text{(B4)}$$

with the initial condition

$$|\Psi(t_0)\rangle\equiv|\psi_R(t_0)\rangle_R|\psi_r(t_0)\rangle_r|\alpha\rangle_1|\beta\rangle_2. \quad \text{(B5)}$$

The subscript $R(r)$ denotes the center-of-mass (relative) motion, as defined in Appendix A 1. The solution is [10]

$$|\psi_R(t)\rangle_R=e^{-iH_R^0(t-t_0)/\hbar}\exp\left(iX_0\int_{t_0}^t F(t')dt'/\hbar\right)\times\exp\left[-\int_{t_0}^t dsK_R(s,t_0)\frac{dK_R^*(s,t_0)}{ds}\right]\times e^{-iK_R(t,t_0)\hat a_R^\dagger}e^{-iK_R^*(t,t_0)\hat a_R}|\psi_R(t_0)\rangle_R, \quad \text{(B6a)}$$

$$|\psi_r(t)\rangle_r=e^{-iH_r^0(t-t_0)/\hbar}\exp\left(id\int_{t_0}^t f(t')dt'/\hbar\right)\times\exp\left[-\int_{t_0}^t dsK_r(s,t_0)\frac{dK_r^*(s,t_0)}{ds}\right]\times e^{-iK_r(t,t_0)\hat a_r^\dagger}e^{-iK_r^*(t,t_0)\hat a_r}|\psi_r(t_0)\rangle_r, \quad \text{(B6b)}$$

where $\hat a_R$ ($\hat a_r$) is the annihilation operator for the $x$ component of the center-of-mass (relative) motion, and

$$K_R(t,t_0)\equiv\frac{1}{\sqrt{2M\hbar\omega}}\int_{t_0}^{t}dt'F(t')e^{i\omega(t'-t_0)}, \quad \text{(B7a)}$$

$$K_r(t,t_0)\equiv\frac{1}{\sqrt{2\mu\hbar\nu}}\int_{t_0}^{t}dt'f(t')e^{i\nu(t'-t_0)}. \quad \text{(B7b)}$$

Now the explicit form of the force term, Eq. (4.9), can be inserted into Eqs. (B7a) and (B7b) through Eq. (A13), to yield

$$K_R(t,t_0)=(\hat{\Pi}_1+\hat{\Pi}_2)K(\omega,t,t_0), \quad \text{(B8a)}$$

$$K_r(t,t_0)=(\hat{\Pi}_2-\hat{\Pi}_1)K(\nu,t,t_0), \quad \text{(B8b)}$$

where

$$K(\omega,t,t_0)\equiv\frac{\sqrt{\pi}}{4}\omega\tau\xi e^{-(\omega\tau/2)^2}I(\omega,t')\Big|_{t_0}^{t}, \quad \text{(B9a)}$$

$$I(\omega,t)\equiv\mathrm{Erf}\left(\frac{t}{\tau}-\frac{i\omega\tau}{2}\right). \quad \text{(B9b)}$$

We take as initial state

$$|\psi_R(t_0)\rangle_R\equiv|\mathbf{N}\rangle_R\equiv|N_X\rangle_X|N_Y\rangle_Y|N_Z\rangle_Z, \quad \text{(B10a)}$$

$$|\psi_r(t_0)\rangle_r\equiv|\mathbf{n}\rangle_r\equiv|n_x\rangle_x|n_y\rangle_y|n_z\rangle_z. \quad \text{(B10b)}$$

During time evolution, the two ions will acquire a state-dependent phase shift

$$\langle\Psi(t)|\Psi(t_0)\rangle\equiv|\langle\Psi(t)|\Psi(t_0)\rangle|e^{i\phi^{\alpha\beta}}, \quad \text{(B11)}$$

which turns out to be given by

$$\phi^{\alpha\beta}=\phi_R^{\alpha\beta}+\phi_r^{\alpha\beta}, \quad \text{(B12a)}$$

$$\phi_R^{\alpha\beta}\approx(\alpha+\beta)^2\xi^2\Phi(\omega)+(\alpha+\beta)\sqrt{\pi}\omega\tau\xi X_0/a_\omega -(N_X+N_Y+N_Z)\omega(t-t_0), \quad \text{(B12b)}$$

$$\phi_r^{\alpha\beta}\approx(\alpha-\beta)^2\xi^2\Phi(\nu)-(\alpha-\beta)\sqrt{\pi}\omega\tau\xi d/a_\omega -[n_x\nu+(n_y+n_z)\nu_\perp](t-t_0), \quad \text{(B12c)}$$

$$\Phi(\omega)\equiv-\pi\omega^2\tau\frac{A^2}{8C}D(t')\Big|_{t_0}^{t}e^{(B/C)^2-(\omega\tau/2)^2}, \quad \text{(B12d)}$$

with

$$A\equiv\mathrm{Im}[I(\omega,t_0)]-iI^*(\omega,0),$$

$$B\equiv\omega\,\mathrm{Re}[I(\omega,t_0)],$$

$$C\equiv2\sqrt{A^2\left(\frac{\omega^2}{2}+\frac{1}{\tau^2}\right)-\frac{A\omega}{\sqrt{\pi}\tau}e^{(\omega\tau/2)^2}+\frac{B^2}{4}},$$

$$D(t)\equiv\mathrm{Erf}\left(\frac{B}{C}+\frac{C}{2A}t\right). \quad \text{(B13)}$$

The equality in Eqs. (B12b) and (B12c) is approximate since the integrals in the exponent of Eqs. (B6a) and (B6b) have been evaluated by means of a saddle-point approximation, giving a very good agreement (relative difference less than $10^{-5}$ with typical parameters as used here) with the exact result, which cannot be evaluated analytically. Finally, from Eqs. (B6a) and (B6b) we obtain

$$\mathcal{O}^{\{n_i\}}(t,t_0)\equiv|\langle\Psi(t)|\Psi(t_0)\rangle|=\mathcal{O}_R^{\{n_i\}}\mathcal{O}_r^{\{n_i\}}, \quad \text{(B14)}$$

where

$$\mathcal{O}_R^{\{n_i\}}=M(-N_X,1,|K_R(t,t_0)|^2)e^{-|K_R(t,t_0)|^2/2}, \quad \text{(B15a)}$$

$$\mathcal{O}_r^{\{n_i\}}=M(-n_x,1,|K_r(t,t_0)|^2)e^{-|K_r(t,t_0)|^2/2}, \quad \text{(B15b)}$$

and $M(a,b,z)$ is the confluent hypergeometric function.

### 3. First-order perturbation theory

Now we want to evaluate the lowest-order corrections that appear when the higher-multipole contributions in the Hamiltonian are taken into account. Following [10], we expand the evolution operator as

$$U(t,t_0)=U_0(t,t_0)+\sum_{j=1}^{\infty}U_j(t,t_0), \quad \text{(B16)}$$

where $U_0(t,t_0)$ is the operator of the unperturbed evolution, already calculated in Appendix B 2, and

$$U_j(t,t_0)\equiv\frac{1}{(i\hbar)^j}\int_{t_0}^{t}dt_j\int_{t_0}^{t_j}dt_{j-1}\cdots\int_{t_0}^{t_2}dt_1U_0(t,t_j) \times H_1U_0(t_j,t_{j-1})H_1U_0(t_{j-1},t_{j-2})\cdots U_0(t_2,t_1) \times H_1U_0(t_1,t_0). \quad \text{(B17)}$$

We are interested in evaluating the diagonal matrix elements $\langle\Psi(t_0)|U(t,t_0)|\Psi(t_0)\rangle$ to first order, according to Eq. (B16). Since $\langle U_0(t,t_0)\rangle$ is given by Eq. (B11), we just need to compute

$$\langle U_1(t,t_0)\rangle=\frac{1}{i\hbar}\int_{t_0}^{t}dt'\mathcal{O}_1^{\alpha\beta}(t,t',t_0)e^{i[\phi_r^{\alpha\beta}(t,t')+\phi_r^{\alpha\beta}(t',t_0)]} =\frac{e^{i\phi_r^{\alpha\beta}(t,t_0)}}{i\hbar}\int_{t_0}^{t}dt'\mathcal{O}_1^{\alpha\beta}(t,t',t_0) \quad \text{(B18)}$$

where the unperturbed phase factorizes, since (as shown in Sec. V A) it does not depend on the initial state, and we have defined

$$\mathcal{O}_1^{\alpha\beta}(t,t',t_0)\equiv|\langle\Psi(t_0)|U_0(t,t')H_1U_0(t',t_0)|\Psi(t_0)\rangle|. \quad \text{(B19)}$$

The exact result, given by Eqs. (B6a) and (B6b), cannot be integrated analytically over time. Instead we adopt the adiabatic approximation, i.e., we assume that the condition (i) of Sec. IV is satisfied. The Hamiltonian then changes slowly

enough so that the system, being in a motional eigenstate at $t=t_0$, follows the changes, being in the corresponding eigenstate at every subsequent time $t$. This means in our case that, if $t_0<0$, $t>0$, and their absolute values are large enough, we will have $|\Psi(t)\rangle\approx|\Psi(t_0)\rangle$. The relative motion wave function of the evolved state is then

$$|\langle\psi_r(t_0)|U_0(t,t')|\mathbf{r}\rangle|\approx|\langle\mathbf{r}|U_0(t',t_0)|\psi_r(t_0)\rangle| \approx\psi_{n_x}(x-f(t)/\mu\nu^2)\psi_{n_y}(y)\psi_{n_z}(z), \tag{B20}$$

where, e.g., $\psi_{n_x}(x)\equiv\langle x|n_x\rangle_x\in\mathbb{R}$. Finally we obtain

$$\langle U_1(t,t_0)\rangle\approx ie^{i\phi_r^{\alpha\beta}}(\Delta^{\alpha\beta}+\Delta'), \tag{B21}$$

where

$$\Delta^{\alpha\beta}\equiv-\frac{\sqrt{\pi}\tau}{\hbar}\frac{\lambda}{d}\sum_{k=3}^{\infty}\left[\frac{a_\nu}{d}\tilde{\xi}(\alpha-\beta)\right]^k\delta_k, \tag{B22a}$$

$$\Delta'\equiv-\frac{t-t_0}{\hbar}\frac{\lambda}{d}\sum_{k=3}^{\infty}\left(\frac{a_\nu}{d}\right)^k\delta_k', \tag{B22b}$$

$$\delta_k\equiv\frac{1}{\sqrt{\pi}\tau(a_\nu\tilde{\xi})^k}\int_{t_0}^{t}dt'\langle\mathbf{n}|\left[P_k\left(x+\frac{\omega^2}{\nu^2}a_\omega\mathcal{F}(t),y,z\right)-P_k(x,y,z)\right]|\mathbf{n}\rangle_r, \tag{B22c}$$

$$\delta_k'\equiv\frac{\langle\mathbf{n}|P_k(x,y,z)|\mathbf{n}\rangle_r}{a_\nu^k}, \tag{B22d}$$

$$\tilde{\xi}\equiv\xi\frac{a_\nu}{a_\omega}\frac{\omega}{\nu}=\frac{\sqrt{2}\xi}{(1-\epsilon)^{3/4}},\quad a_\nu\equiv\sqrt{\hbar/\mu\nu}. \tag{B22e}$$

From Eqs. (B16) and (B21) it follows that, to first order,

$$\langle U(t,t_0)\rangle\approx\langle U_0(t,t_0)+U_1(t,t_0)\rangle =\langle U_0(t,t_0)\rangle\left[1+i\frac{\Delta^{\alpha\beta}+\Delta'}{|\langle U_0(t,t_0)\rangle|}\right], \tag{B23}$$

which is equivalent to Eq. (5.5), given that $|\Delta^{\alpha\beta}+\Delta'|=|\langle U_1(t,t_0)\rangle|\ll|\langle U_0(t,t_0)\rangle|\approx1$. The internal-state-independent part $\Delta'$ cancels out when computing the gate phase Eq. (2.8), as well as the terms of odd $k$ in $\Delta^{\alpha\beta}$, due to the summation over the internal states. The adimensional quantities $\delta_k$ and $\delta_k'$ do not depend either on the internal state or on time, but just on the relative motional state. We will now calculate them for $k=3,4$. To be precise, we should not use the eigenstates $|\mathbf{n}\rangle_r$ of $H_r^0$, as is done in Eq. (B22d), but rather those of the full Hamiltonian $H_r$. However, as we will demonstrate in the next section, the corrections are of $o((a_\omega/d)^3)$ and therefore we will consistently not take them into account in the present calculation. The relevant matrix elements are

$$\langle n|x|n'\rangle=\frac{a_\nu}{\sqrt{2}}(\delta_{n',n-1}\sqrt{n}+\delta_{n',n+1}\sqrt{n+1}), \tag{B24a}$$

$$\langle n|x^2|n'\rangle=\frac{a_\nu^2}{2}[\delta_{n',n-2}\sqrt{n(n-1)}+\delta_{n',n}(2n+1)+\delta_{n',n+2}\sqrt{(n+1)(n+2)}], \tag{B24b}$$

$$\langle n|x^3|n'\rangle=\frac{a_\nu^3}{2^{3/2}}[\delta_{n',n-3}\sqrt{n(n-1)(n-2)}+3\delta_{n',n-1}n+3\delta_{n',n+1}(n+1)^{3/2}+\delta_{n',n+3}\sqrt{(n+1)(n+2)(n+3)}], \tag{B24c}$$

$$\langle n|x^4|n'\rangle=\frac{a_\nu^4}{4}\{\delta_{n',n-4}\sqrt{n(n-1)(n-2)(n-3)}+2\delta_{n',n-2}\times(2n+1)\sqrt{n(n-1)}+3\delta_{n',n}[2n(n+1)+1]+2\delta_{n',n+2}(2n+3)\sqrt{(n+1)(n+2)}+\delta_{n',n+4}\sqrt{(n+1)(n+2)(n+3)(n+4)}\}. \tag{B24d}$$

Hence

$$\delta_3=-\frac{1}{\sqrt{3}}-\frac{3}{2\tilde{\xi}^2}[2n_x+1-\tilde{\nu}(n_y+n_z+1)], \tag{B25a}$$

$$\delta_4=\frac{1}{2}+\frac{3}{\sqrt{2}\tilde{\xi}^2}[2n_x+1-\tilde{\nu}(n_y+n_z+1)], \tag{B25b}$$

$$\delta_3'=0, \tag{B25c}$$

$$\delta_4'=\frac{3}{4}[2n_x(n_x+1)+1]-\frac{3}{2}\tilde{\nu}(2n_x+1)(n_y+n_z+1)+\frac{3}{16}\tilde{\nu}^2[n_y(3n_y+5)+n_z(n_z+5)+4(1+n_yn_z)], \tag{B25d}$$

where $\tilde{\nu}\equiv\nu/\nu_\perp$.

#### 4. Perturbative corrections to the eigenstates

Since in our case the perturbation $H_1$ is static, its effect on the initial eigenstates of the system must be taken into account. In this section we show how to do that in second-order perturbation theory. Our problem is to compute the eigenstates of the initial relative motion Hamiltonian

$$H_r(t_0)=H_r^0+H_1=H_r^0+\epsilon H_r^1, \tag{B26}$$

whereby the external force is vanishing at the initial time, and

$$H_r^1 \equiv \frac{\hbar\omega}{2}\frac{d^2}{a_\omega^2}\sum_{k=3}^{\infty}\frac{P_k(x,y,z)}{d^k}. \tag{B27}$$

Therefore we make a perturbative expansion in the small parameter $\epsilon$. So we write the eigenstates of $H_r$ (omitting throughout this section the subscript $r$) as

$$|\mathbf{n}(\epsilon)\rangle = \sum_{i=0}^{\infty}\epsilon^i|\mathbf{n}^{(i)}\rangle, \tag{B28}$$

where the first terms are

$$|\mathbf{n}^{(1)}\rangle = \sum_{\mathbf{m}\neq\mathbf{n}}\frac{\langle\mathbf{m}^{(0)}|H_r^1|\mathbf{n}^{(0)}\rangle}{E_{\mathbf{n}}^{(0)}-E_{\mathbf{m}}^{(0)}}|\mathbf{m}^{(0)}\rangle, \tag{B29a}$$

$$|\mathbf{n}^{(2)}\rangle = \sum_{\mathbf{l},\mathbf{m}\neq\mathbf{n}}\frac{\langle\mathbf{m}^{(0)}|H_r^1|\mathbf{l}^{(0)}\rangle\langle\mathbf{l}^{(0)}|H_r^1|\mathbf{n}^{(0)}\rangle}{(E_{\mathbf{n}}^{(0)}-E_{\mathbf{m}}^{(0)})(E_{\mathbf{n}}^{(0)}-E_{\mathbf{l}}^{(0)})}|\mathbf{m}^{(0)}\rangle, \tag{B29b}$$

and $|\mathbf{n}^{(0)}\rangle$ are the eigenstates of $H_r^0$, with eigenenergies $E_{\mathbf{n}}^{(0)}$. The $k$th term in $H_r^1$ gives a contribution of order $\sim(\hbar\omega/2)\times(a_\omega/d)^{k-2}$. Since we want to neglect corrections of order $o((a_\omega/d)^3)$, we need to go up to $k=4$ in the expansion of $H_r^1$. But from Eqs. (A6a) and (A6b) it is straightforward to see that $\langle\mathbf{m}^{(0)}|P_{3,4}(x,y,z)|\mathbf{n}^{(0)}\rangle$ for $\mathbf{m}\neq\mathbf{n}$. It follows that

$$|\mathbf{n}(\epsilon)\rangle = |\mathbf{n}^{(0)}\rangle + o((a_\omega/d)^3), \tag{B30}$$

and therefore, as already anticipated in the previous section, for the purpose of the present calculation we can consistently use the eigenstates of the unperturbed Hamiltonian $H_r^0$.

#### 5. Numerical computation

The goal of this section is to transform the Schrödinger equation for the two-particle wave function into a system of first-order differential equations for the time dependence of its projections over the initial eigenstates, better suitable for numerical handling. Since the problem has cylindrical symmetry around the $x$ axis, the transverse coordinates always appear as powers of $\rho\equiv\sqrt{y^2+z^2}$. Thus the original three-dimensional problem is equivalent to a two-dimensional one. We expand the wave function (omitting for simplicity the subscript $r$) as

$$|\psi(t)\rangle = \sum_{n,l=0}^{\infty}c_{nl}(t)\times\exp\left\{\frac{i}{\hbar}\left[d\int_{t_0}^{t}f(t')dt' - \hbar(n\nu + l\nu_\perp + 1)t\right]\right\}|nl\rangle, \tag{B31}$$

where $|nl\rangle\equiv|n\rangle_x|l\rangle_\perp$; the $|n\rangle_x(|l\rangle_\perp)$ are the eigenstates of $H_x(H_\perp)$. From Eq. (B4) it follows that

$$\begin{aligned}\dot{c}_{nl} &= \frac{i}{\hbar}\sum_{n',l'=0}^{\infty}c_{n'l'}(t)e^{i[(n-n')\nu+(l-l')\nu_\perp]t}\times\langle nl|[f(t)x-H_1]|n'l'\rangle \\ &= \frac{i}{\hbar}\left[\frac{a_\nu}{\sqrt{2}}f(t)(\sqrt{n}e^{i\nu t}c_{n-1,l}+\sqrt{n+1}e^{-i\nu t}c_{n+1,l}) + \frac{\lambda}{d}\sum_{k=3}^{\infty}\left(\frac{a_\nu}{\sqrt{2}d}\right)^k C_{nl}^{(k)}\right],\end{aligned} \tag{B32}$$

where the coefficients $C_{nl}^{(k)}$ correspond to the $k$th term in Eq. (A9); in particular,

$$\begin{aligned}C_{nl}^{(3)} &= \sqrt{n(n-1)(n-2)}e^{i3\nu t}c_{n-3,l}+3n^{3/2}e^{i\nu t}c_{n-1,l}+3(n+1)^{3/2}e^{-i\nu t}c_{n+1,l}+\sqrt{(n+1)(n+2)(n+3)}e^{-i3\nu t}c_{n+3,l} \\ &- \frac{3\tilde{\nu}}{2}[\sqrt{nl(l-1)}e^{i(\nu+2\nu_\perp)t}c_{n-1,l-2}+\sqrt{n(l+1)(l+2)}e^{i(\nu-2\nu_\perp)t}c_{n-1,l+2}+(2l+1)(\sqrt{n}e^{i\nu t}c_{n-1,l} \\ &+ \sqrt{n+1}e^{-i\nu t}c_{n+1,l})+\sqrt{(n+1)l(l-1)}e^{-i(\nu-2\nu_\perp)t}c_{n+1,l-2}+\sqrt{(n+1)(l+1)(l+2)}e^{-i(\nu+2\nu_\perp)t}c_{n+1,l+2}],\end{aligned} \tag{B33a}$$

$$\begin{aligned}C_{nl}^{(4)} &= -\sqrt{n(n-1)(n-2)(n-3)}e^{4i\nu t}c_{n-4,l}+\sqrt{n(n-1)}e^{2i\nu t}\{3\tilde{\nu}[\sqrt{l(l-1)}e^{2i\nu_\perp t}c_{n-2,l-2}+\sqrt{(l+1)(l+2)}e^{-2i\nu_\perp t}c_{n-2,l+2} \\ &+ (2l+1)c_{n-2,l}]-2(2n-1)c_{n-2,l}\}-\frac{3\tilde{\nu}^2}{8}\sqrt{l(l-1)(l-2)(l-3)}e^{4i\nu_\perp t}c_{n,l-4}+3\tilde{\nu}\sqrt{l(l-1)} \\ &\times\left[(2n+1)-\frac{\tilde{\nu}}{4}(2l-1)\right]e^{2i\nu_\perp t}c_{n,l-2}-\left\{\frac{9\tilde{\nu}^2}{8}[2l(l+1)+1]-3\tilde{\nu}(2n+1)(2l+1)+3[2n(n+1)+1]\right\}c_{nl} \\ &- \frac{3}{4}\tilde{\nu}\sqrt{(l+1)(l+2)}[\tilde{\nu}(2l+3)-4(2n+1)]e^{-2i\nu_\perp t}c_{n,l+2}-\frac{3\tilde{\nu}^2}{8}\sqrt{(l+1)(l+2)(l+3)(l+4)}e^{-4i\nu_\perp t}c_{n,l+4}\end{aligned}$$

$$+\sqrt{(n+1)(n+2)}e^{-2i\nu t}\{3\tilde{\nu}[(2l+1)c_{n+2,l}+\sqrt{(l+1)(l+2)}e^{-2i\nu_\perp t}c_{n+2,l+2}\sqrt{l(l-1)}e^{2i\nu_\perp t}c_{n+2,l-2}]-2(2n+3)c_{n+2,l}\}$$
$$-\sqrt{(n+1)(n+2)(n+3)(n+4)}e^{-4i\nu t}c_{n+4,l}. \tag{B33b}$$

Excitations higher than a certain level should be absent as long as we are in an adiabatic regime. Thus in Eq. (B32) we neglect the coefficients above a certain $N$. We have checked that the result is independent of the cutoff.

### 6. Fidelity

The goal of this section is to evaluate the gate operation fidelity in the full three-dimensional quantum-mechanical framework. The overall phase $\Theta$ appearing in Eq. (5.13) can be computed from Eqs. (B12a)–(B12d) and (B22a)–(B22d), as

$$\Theta \approx 2\omega\left\{\sqrt{\pi}\xi\tau\frac{X_0}{a_\omega}-\left[\sum_{i=1}^{6} n_i+\epsilon\sum_{k=3}^{\infty}\left(\frac{a_\omega}{d}\right)^k\delta_k'\right](t-t_0)\right\}, \tag{B34}$$

where $\delta_4'$ is defined in Eq. (B25d), and it has been taken into account that $\epsilon \ll 1$. In the ideal case, according to Eq. (2.1) for $\vartheta=\pi$, the gate operation transforms the initial internal state $|\chi\rangle$ into

$$|\chi'\rangle=\sum_{\alpha,\beta=0}^{1}(-1)^{\alpha\beta}c_{\alpha\beta}|\alpha\rangle_1|\beta\rangle_2. \tag{B35}$$

In a more realistic situation the initial total density operator $\sigma_T$ at a temperature $T$ is given by

$$\sigma_T=\rho_T(t_0)\otimes|\chi\rangle\langle\chi|, \tag{B36}$$

where $\rho_T(t_0)$ is defined in Eq. (5.4), and we recall that $\omega \approx \nu \approx \nu_\perp$. After the gate operation we have

$$\sigma_T'=\sum_{\alpha,\beta,\alpha',\beta'}c_{\alpha\beta}c^*_{\alpha'\beta'}G_{\alpha\beta}\rho_T(t_0)G^\dagger_{\alpha'\beta'}|\alpha\rangle_1 \times\langle\alpha'|\otimes|\beta\rangle_2\langle\beta'|, \tag{B37}$$

where $G_{\alpha\beta}\equiv\langle\alpha\beta|G|\alpha\beta\rangle$, and the gate operator $G$ is defined in Eq. (5.13). As already stated in Sec. V A, because of adiabaticity, the motional state after the gate operation is unchanged, i.e., $G_{\alpha\beta}\rho_T(t_0)G^\dagger_{\alpha'\beta'}\approx\rho_T(t_0)$. If $\theta=\pi$, the minimum fidelity $F(T)$, given by Eq. (2.5), is

$$F(T)=\min_{\{c_{\alpha\beta}\}}(1-\gamma)^6\prod_{i=1}^{6}\sum_{n_i=1}^{\infty}\gamma^{n_i}\langle n_i|[(|c_{00}|^2+|c_{11}|^2)^2 +2(|c_{00}|^2+|c_{11}|^2)(|c_{01}|^2+|c_{10}|^2)\cos(\Delta\theta) +(|c_{01}|^2+|c_{10}|^2)^2]|n_i\rangle$$
$$=\frac{(1-\gamma)^3}{2}\prod_{i=1}^{3}\sum_{n_i=1}^{\infty}\gamma^{n_i}\langle n_i|[1+\cos(\Delta\theta)]|n_i\rangle$$
$$\approx 1-\frac{6^3\theta_{\rm cl}^2}{(1+\epsilon^5)(1-\epsilon^2/4)}\left(\frac{a_\omega}{d}\right)^4\frac{e^{-\hbar\nu/k_BT}}{(1-e^{-\hbar\nu/k_BT})^2}, \tag{B38}$$

where the minimization over the coefficients $\{c_{\alpha\beta}\}$ has been carried out exactly as in Appendix A 2. Here, only the relative motion comes into play because $\Delta\theta$ is independent of the center-of-mass motion, and $\cos(\Delta\theta)$ has been expanded up to $o(\Delta\theta^3)$. Hence Eq. (5.14) follows, by taking into account that $\epsilon \ll 1$ and $\theta_{\rm cl}\approx\theta=\pi$, and expanding in a Taylor series for $\hbar\omega \ll k_BT$.

### 7. Many-ion calculation

In this section we simply give the definitions of the parameters appearing in Eq. (5.18):

$$\varepsilon_i\equiv\frac{\omega_i^2}{\omega^2}\tilde{x}_i^2-\frac{\epsilon}{2}d^2\mathcal{H}_{n-i}, \tag{B39a}$$

$$\omega_i\equiv\omega\sqrt{1+\epsilon\eta_i},\quad \tilde{x}_i\equiv\frac{d}{2}\frac{\epsilon\eta_i'}{1+\epsilon\eta_i}, \tag{B39b}$$

$$\eta_i\equiv\frac{1}{2}\sum_{j=1}^{N}\frac{1-\delta_{ij}}{|i-j|^3}=\frac{1}{4}[\psi^{(2)}(i)+\psi^{(2)}(N+1-i)+\zeta(3)], \tag{B39c}$$

$$\eta_i'\equiv\frac{1}{2}\sum_{j=1}^{N}\frac{i-j}{|i-j|^3}=\frac{1}{2}[\psi^{(1)}(N+1-i)-\psi^{(1)}(i)], \tag{B39d}$$

where $\mathcal{H}_k$ is the harmonic number and $\psi^{(k)}(z)$ the polygamma function of order $k$, and $\zeta(s)$ the Riemann zeta function. It is

$$\max_{i,n}|\eta_i|=\zeta(3)\approx 1.2,\quad \max_{i,n}|\eta_i'|=\frac{\pi^2}{12}\approx 0.82. \tag{B40}$$

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