Entangling ions in arrays of microscopic traps

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(Dated: March 31, 2022)

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.

PACS numbers: 03.67.-a, 42.50.-p

I. INTRODUCTION

The possibilities offered by quantum mechanical systems for efficient information processing have stimulated in recent years the rise of an entirely new field of research.\textsuperscript{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 remains still at a less advanced level, as far as physical implementation is concerned. Different systems are being proposed as candidates for this purpose\textsuperscript{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 been already 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\textsuperscript{3}, and requires an error probability for elementary operations below a certain threshold (of the order of \( 10^{-4} \)). Hence the need for new 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 – of manufacturing 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 imperfections. 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 already proposed several schemes, based on different interactions – collisional interactions between neutral atoms in optical lattices\textsuperscript{4} and magnetic microtraps\textsuperscript{5}, or dipole-dipole interactions between Rydberg-excited atoms\textsuperscript{6}. Here we deal with electrostatic interaction between ions\textsuperscript{7} in arrays of microscopic traps\textsuperscript{8}.

In this paper we describe the conditional dynamics for 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\textsuperscript{9}. 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). To 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 eventually compared with the ideal state we aim to obtain. The fidelity of gate operation is evaluated, in this classical model, as the overlap of the real and the ideal state we aim to obtain. The fidelity of 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 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 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 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 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 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 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 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 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 after gate
fined 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 particles’ internal states. One basic building block towards multi-qubit entanglement operations is the phase gate between two qubits – a transformation which rotates by a certain phase just one component of logical states:

\[
\begin{align*}
|0\rangle|0\rangle & \rightarrow |0\rangle|0\rangle, \\
|0\rangle|1\rangle & \rightarrow |0\rangle|1\rangle, \\
|1\rangle|0\rangle & \rightarrow |1\rangle|0\rangle, \\
|1\rangle|1\rangle & \rightarrow e^{i\vartheta}|1\rangle|1\rangle.
\end{align*}
\]

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

\[
H_{\text{int}} = \Delta E(t)|1\rangle\langle 1| \otimes |1\rangle\langle 1|,
\]

acting over a time \( \tau \) such that

\[
\int_0^\tau \Delta E(t')dt' = \vartheta.
\]

However, it is not straightforward to realize in practice an interaction between two particles which 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. (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 leaving eventually the external degrees of freedom practically unaffected. This is described a Hamiltonian of the form

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

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. (1), with the gate that can be actually realized by the physical process described by Eq. (4).

The figure of merit is the minimum fidelity \( F \), given by

\[
F = \min_{\chi} \text{tr}_{\text{ext}} \langle \chi' | \sigma' | \chi' \rangle,
\]

where \( \text{tr}_{\text{ext}} \) denotes the trace over the external degrees of freedom, \( |\chi\rangle = \sum_{\alpha\beta} c_{\alpha\beta} |\alpha\rangle_1 |\beta\rangle_2 \) is a generic two-ion internal state, \( |\chi'\rangle \) is the state obtained from \(|\chi\rangle\) via the transformation Eq. (1), and \( \sigma' \) is the total density matrix, including external degrees of freedom, after the evolution dictated by the Hamiltonian Eq. (4), starting from an initial state

\[
\sigma = \rho_1(t_0) \otimes \rho_2(t_0) \otimes |\chi\rangle \langle \chi|,
\]

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 that the external degrees of freedom factorize after the gate operation, and that the evolution operator

\[
U(t, t_0) = T \exp \left\{ -i \int_{t_0}^t H(t', \mathbf{x}_1, \mathbf{x}_2)dt' \right\}
\]

has the only effect to induce 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 App. B), leaving us with the gate phase

\[
\vartheta = \varphi^{00} - \varphi^{01} - \varphi^{10} + \varphi^{11}.
\]

In a real situation, the starting point will be rather 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) \( \bar{r}_i \) \((1 \leq i \leq N)\). 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 \( F_i(t) \), depending on its internal state \( \alpha_i \in \{0, 1\} \) as in Eq. (4). The Hamiltonian is

\[
H = \sum_{i=1}^N H_i + \sum_{i<j}^N H_{ij},
\]
We can rewrite the Hamiltonian in Eq. (4) as

\[ H_i \equiv \frac{p_i^2}{2m} + \frac{1}{2} m \omega_t^2 (r_i - \bar{r}_i)^2 - F_i(t) \cdot r_i, \quad (10a) \]

\[ H_{ij} \equiv \frac{q_e^2}{4\pi\varepsilon_0} \frac{1}{|r_i - r_j|}, \quad (10b) \]

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:

\[ F_i(t) = \sum_{\alpha=0}^{1} |\alpha\rangle_i \langle \alpha| \otimes F^\alpha(t). \quad (11) \]

We can rewrite the Hamiltonian in Eq. (4) as

\[ H^{\alpha_1\alpha_2}(t, x_1, x_2) = \sum_{i=1}^{2} \left\{ \frac{p_i^2}{2m} + \frac{m \omega_t^2}{2} |x_i - x^\alpha_i(t)|^2 \right\} - \frac{F^\alpha(t)^2}{2} \]

\[ + \frac{q_e^2}{4\pi\varepsilon_0} \frac{1}{|d + x_2 - x_1|}, \]

where we have defined \( x_1 \equiv r_1 + d/2, \ x_2 \equiv r_2 - d/2, \ x^\alpha(t) \equiv F^\alpha(t)/(m\omega_t^2), \) and \( d \) is the equilibrium inter-particle separation. We assume the external force to act along its direction, and we choose the simple state dependence \( F^\alpha(t) \equiv (\alpha \omega_t F(t)/a_\alpha, 0, 0) \). Here \( a_\omega \equiv \sqrt{\hbar/m\omega} \) is the quantum harmonic oscillator ground-state width. Hence the adimensional quantity \( F(t) \) 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 \( |\alpha\rangle_i \); indeed, we have \( x^\alpha(t) = \alpha a_\omega (F(t), 0, 0) \). With the above choice for the state dependence of the force, the last term in the first row at right-hand side of Eq. (12) will not contribute to the gate phase Eq. (4), since the corresponding terms cancel each other in the sum \( \sum_{\alpha,\beta} (-1)^{\alpha+\beta} \varphi^{\alpha\beta} \). Since the interaction only depends 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 App. A) as \( H(t) = H_R(t) + H_r(t) \), where

\[ H_R(t) = H_R^0 - \hat{F}(t) \cdot \left( R + \frac{\bar{r}_1 + \bar{r}_2}{2} \right), \quad (13a) \]

\[ H_r(t) = H_r^0 - \hat{f}(t) \cdot (r + d) + H_1, \quad (13b) \]

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 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 \( d \). 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

\[ |\chi_{cl}(t_0)\rangle = \sum_{\alpha,\beta=0}^{1} c_{\alpha\beta}|\alpha\rangle_1 |\beta\rangle_2 \quad (14) \]

and by the external classical trajectories \( x^{\alpha\beta}(t) \) of the two ions, dictated by the Hamiltonian Eq. (4). Here, by \( \alpha = \alpha_1 (\beta = \alpha_2) \) we mean the internal state of the first (second) particle. Indeed, 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

\[ V^{\alpha\beta}(t) = \frac{q_e^2}{4\pi\varepsilon_0} \frac{1}{|d + x^{\alpha\beta}_2(t) - x^{\alpha\beta}_1(t)|} \]

\[ = \frac{q_e^2}{4\pi\varepsilon_0 d} \sum_{n=0}^{\infty} \left[ \frac{x^{\alpha\beta}_1(t) - x^{\alpha\beta}_2(t)}{d} \right]^n. \quad (15) \]

We then define the evolved internal state as

\[ |\chi_{cl}(t)\rangle = \sum_{\alpha,\beta} c_{\alpha\beta}|\alpha\rangle_1 |\beta\rangle e^{i\varphi_{cl}^{\alpha\beta}}, \quad (16) \]

where

\[ \varphi_{cl}^{\alpha\beta} = -\frac{1}{\hbar} \int_{t_0}^{t} V^{\alpha\beta}(t')dt'. \quad (17) \]

Now we make the following assumptions: (i) the force acts slowly over the harmonic oscillator time scale \( \omega^{-1} \),
i.e. $|\mathcal{F}| \ll \omega$; (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 intra-well oscillations (if any) is negligible with respect to the inter-well distance, i.e. $E_i \ll m\omega^2d^2/2$. The first three conditions can be fulfilled by construction, the last one requires in principle the motion to be cooled. Assumption (i) amounts to neglecting non-adiabatic terms in the trajectories (e.g., 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 intra-well motion to be basically unaffected by the higher-order multipole terms in the expansion of the Coulomb interaction, Eq. (15). 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 App. B).

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

\[
x_i(t_0) = \Delta x_i^{E_i}(t_0) \equiv \sqrt{\frac{2E_i}{m\omega^2}} \cos[\tilde{\omega}(t_0 - t_i)], \quad (18a)
\]

\[
\dot{x}_i(t_0) = -\sqrt{\frac{2E_i}{m}} \sin[\tilde{\omega}(t_0 - t_i)] \quad (18b)
\]

(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. (15) — namely, $\tilde{\omega} \equiv \omega \sqrt{1 + \varepsilon/\omega}$, where

\[
\varepsilon \equiv \frac{q^2}{\pi \varepsilon_0 m\omega^2 d^3} \quad (19)
\]

is essentially twice the ratio of the Coulomb energy $q^2/(4\pi\varepsilon_0d)$ and the energy of the second ion with respect to the first trap $m\omega^2d^2/2$. Under the approximations discussed above, we can write the trajectories $x_i^{\alpha\beta}(t)$ as

\[
x_i^{\alpha_1\alpha_2}(t) \approx x_i^{\alpha_1}(t) + \Delta x_i^{E_i}(t) \quad (20)
\]

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 so to speak to two different trapping potentials, as seen in Fig. 3.

![Gate operation dynamics for two classical particles oscillating with energies $E_i$. The state-selective trap displacements $x_i^{E_i}(t)$ and the intra-well oscillations $\Delta x_i^{E_i}(t)$ are shown.](image)

B. Gate phases

We can write the phases Eq. (17) as

\[
\phi_{cl}^{\alpha\beta} = \phi_{cl}^{\alpha\beta} + \delta\phi^{\alpha\beta}, \quad (21)
\]

where $\phi_{cl}^{\alpha\beta}$ 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 to specify the time dependence of the trap displacement. We choose the Gaussian form

\[
\mathcal{F}(t) \equiv \xi e^{-t/(\tau)^2}. \quad (22)
\]

Let us first consider the case where both particles are in their motional ground state. We insert Eq. (21) for $E_i = 0$, through Eq. (15), into Eq. (17), and obtain

\[
\phi_{cl}^{\alpha\beta} = -(\alpha - \beta)^2 \sqrt{\frac{\pi}{8}} \xi^2 \tilde{\omega} \tau \sum_{n=0}^{\infty} \frac{(\alpha - \beta)\xi a_\omega/d}{\sqrt{2(n+1)}} n^{-1}. \quad (23)
\]

In the evaluation of the ground-state phase $\phi_{cl}^{\alpha\beta}$, Eq. (23), the complete Coulomb potential Eq. (15) 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 $2\tau/\omega$ (so that the motional state is left unchanged after gate operation), and find

\[
\delta\phi^{\alpha\beta} = 3(\alpha - \beta) \sqrt{\frac{\pi}{8}} \xi^2 \tilde{\omega} \tau \left\{ \frac{1}{\sqrt{2}\xi} \frac{a_\omega}{d} + (\alpha - \beta) \left( \frac{a_\omega}{d} \right)^2 \right\} \times \left[ \frac{1}{h\tilde{\omega}} \left\{ E_1 + E_2 + 2\sqrt{E_1E_2}\cos[\tilde{\omega}(t_1 - t_2)] \right\} + a(\alpha a_\omega/d)^3 \right] \quad (24)
\]

where it has been taken into account that $\omega \tau \gg 1$. The two terms under square brackets in Eq. (24) come from terms in the Coulomb potential with $n = 3$ and $n = 4$ in Eq. (15), respectively. This means that no thermal correction is to be expected if only harmonic contributions to the potential (i.e., with $n \leq 2$) are included.
Indeed, in this case the spurious interaction phases, due to the oscillations in the ions’ positions, are averaged out when integrating on 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 it will be shown analytically in Sec. A. Now, the classical analogue of the gate phase Eq. (7) can be written as

\[
\theta_{\text{cl}} = \sum_{\alpha, \beta} (-1)^{\alpha + \beta} \sqrt{\omega_t} - \frac{c_{\alpha \beta} a_{\omega}}{d^2} \left[ \left( \frac{\xi}{\sqrt{\beta}} \right)^2 + \frac{6k_B T}{\hbar \omega} \right] \delta_{\alpha \beta} + o\left( \frac{a_{\omega}}{d^2} \right).
\]

Indeed, 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. (11), we require that \( \langle \Phi_{\text{cl}} \rangle = \pi \). So the reference state, representing the ideal evolution, is chosen as

\[
|\chi_{\text{cl}}^\prime\rangle = \sum_{\alpha \beta} c_{\alpha \beta} |\alpha\rangle |\beta\rangle e^{i \langle \Phi_{\text{cl}}^{\alpha \beta} \rangle}.
\]

The real evolved state, Eq. (16), can be written as

\[
|\delta \chi_{\text{cl}}\rangle = \sum_{\alpha \beta} c_{\alpha \beta} |\alpha\rangle |\beta\rangle \left( e^{i \Phi_{\text{cl}}^{\alpha \beta} - e^{i \langle \Phi_{\text{cl}}^{\alpha \beta} \rangle} \right)
\]

In our classical model, we are treating our particles’ external degrees of freedom classically. Therefore, in the evaluation of the fidelity Eq. (9), instead of tracing over the motional eigenstates we should average over the possible classical trajectories. Thus

\[
F_{\text{cl}} = \min_{\chi} \left\langle \left( \chi_{\text{cl}} | \chi_{\text{cl}}(t) \right) \left/ \left( \chi_{\text{cl}} | \chi_{\text{cl}} \right) \right\rangle \right. \left. \right\rangle
\]

\[
= \min_{\chi} \left\langle \left| 1 + \left( \chi_{\text{cl}}(t) | \delta \chi_{\text{cl}} \right)^2 \right| \right. \left. \right\rangle
\]

\[
\left. \left( \sum_{\alpha, \beta = 0}^1 \left| c_{\alpha \beta} \right|^2 e^{-i \langle \Phi_{\text{cl}}^{\alpha \beta} \rangle} \right|^2 \right) \left. \right\rangle
\]

\[
1 - \left( \frac{6k_B T}{\hbar \omega} \right)^2 \left( \frac{a_{\omega}}{d} \right)^2 - 2 \left( \frac{a_{\omega}}{d} \right)^4
\]

\[
+ o\left( \frac{a_{\omega}}{d} \right)^5.
\]

as is discussed in detail in App. 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 \( k = 0 \). We will show later (Sec. V E) how this can be done in practice – here we would like to give a classical estimate \( F_{\text{cl}}' \) of the improved gate fidelity. The calculation is performed in App. A 2 as well, and the result is

\[
F_{\text{cl}}' (T) = 1 - \left( \frac{6k_B T}{\hbar \omega} \right)^2 \left( \frac{a_{\omega}}{d} \right)^4 + o\left( \frac{a_{\omega}}{d} \right)^5.
\]

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 by a wavefunction (see Fig. 3) which evolves according to the Hamiltonian Eq. (4). To better understand its structure, it is useful to write

\[ H^{\alpha\beta}(t, \mathbf{x}_1, \mathbf{x}_2) \equiv H^{\alpha\beta}(t, \mathbf{x}_1^\alpha(t), \mathbf{x}_2^\beta(t)) + H_c^{\alpha\beta}(t, \mathbf{x}_1, \mathbf{x}_2). \]

(33)

Here the \( \mathbf{x}_j \) are the ion position operators, and the c-numbers \( \mathbf{x}_j^\alpha(t) \) denote the centers of the initial motional wavefunctions as determined by the trap (see Sect. I). To second order in the expansion Eq. (5), the first term at the right-hand side of Eq. (33) gives rise to the same contribution to the phase already calculated in lowest order in the classical model, namely \( \theta_{cl} \) given in Eq. (26). 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 \( H_c^{\alpha\beta} \), while multipole corrections get a contribution also from \( H^{\alpha\beta}(t, \mathbf{x}_1^\alpha(t), \mathbf{x}_2^\beta(t)) \). In order to minimize such corrections, we choose to operate in the adiabatic regime, given by condition (i) in Sect. I, i.e. we assume \( \omega \tau \gg 1 \). We study the dynamics in the center-of-mass and relative coordinate system, as given by Eqs. (13a) and (13b). 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.

A. Unperturbed forced oscillator

When we put \( H_1 = 0 \) and take \( F(t) \) as in Eq. (22), the solution to Eq. (24) can be written explicitly (14). This is done in App. B2. The gate phase turns out to be, in this approximation,

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

(34)

where

\[ \Phi(\omega) \equiv -3 \left[ \int_{t_0}^t ds K(s, t_0) \frac{dK^*(s, t_0)}{ds} \right], \]

(35a)

\[ K(t, t_0) \equiv \frac{1}{m\hbar} \int_{t_0}^t dt' F(t') e^{i\omega(t'-t_0)}. \]

(35b)

Explicit expressions for \( \phi^{\alpha\beta} \) and for \( \Phi(\omega) \) are given in Eqs. (112a)-(112d). In the limit \( \omega \gg 1 \), we obtain \( \Phi(\omega) \approx -\sqrt{\pi/2}\omega t \). By expanding Eq. (24) up to first order in \( \epsilon \), we retrieve \( \theta \approx \theta_{cl} \) as given by Eq. (26). 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

\[ \rho_T(t_0) \equiv \frac{e^{-H(t_0)/kB_T}}{Z} \approx (1 - \gamma)^6 \sum_{n=1}^\infty \gamma^ni_1\cdots ni, \]

(36)

corresponding to a thermal distribution at a temperature \( T \). Here the canonical partition function \( Z \equiv \text{tr} \left\{ e^{-H(t_0)/kB_T} \right\} \), \( \gamma \equiv \exp(-\hbar/\omega kB_T) \), \( \{n_i\}_{i=1}^6 \equiv \{n_x, n_y, n_z, N_X, N_Y, N_Z\} \), and the \( |n\rangle_{X,Y,Z} \) are the eigenstates of \( H_T^x \) (\( H_T^y \)) along each direction. To optimize the gate fidelity (see Sect. II), we need basically 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 Sect. IV. In fact, in this case, the overlap \( \mathcal{O}^{(\alpha\beta)}(t, t_0) \) between the
In order to check the validity of the perturbative expression Eq. (38), we solved numerically the Schrödinger equation for the relative motion, taking into account cubic and quartic interaction terms, explicitly given by Eqs. (A6a) and (A6b) respectively. The calculation is described in App. B.5, and results are shown in Fig. 5. In particular we find that the cubic corrections cancel indeed each other, and that the quartic corrections have the same order of magnitude as predicted by Eq. (38).

C. Numerical computation

In order to check the validity of the perturbative expression Eq. (38), we solved numerically the Schrödinger equation for the relative motion, taking into account cubic and quartic interaction terms, explicitly given by Eqs. (A6a) and (A6b) respectively. The calculation is described in App. B.5, and results are shown in Fig. 5. In particular we find that the cubic corrections cancel indeed each other, and that the quartic corrections have the same order of magnitude as predicted by Eq. (38). From Eq. (44) we obtain θ = π with ω = 2π × 1 MHz, \( \bar{\delta} = 20 \mu \text{m} \), ξ = 0.7 and τ = 41.1069 \( \mu \)s. These results were confirmed by the numerical computation up to 40 initial excitations in each direction, always giving unity overlap of the final motional state on the initial one. Indeed, with \( t = -t_0 = 150 \mu \)s, even starting e.g. with the (10\^-6 \( \mu \)s) oscillator excited state, Eq. (31) 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 \( \theta_{cl} \approx 104 \pi \).

D. Gate fidelity

The gate phase θ cannot be measured directly, since the higher-order corrections arising from the Coulomb potential depend both on the intern 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. (32a). This implies that it is possible to obtain a cancellation of the odd-order corrections, by applying a π-pulse \( \bar{R} = |0\rangle \langle 1| + |1\rangle \langle 0| \) 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

\[
\begin{align*}
|0\rangle|0\rangle & \rightarrow e^{i\varphi_{00}}|1\rangle|1\rangle & \rightarrow e^{i(\varphi_{00}+\varphi_{11})}|0\rangle|0\rangle \\
|0\rangle|1\rangle & \rightarrow e^{i\varphi_{01}}|1\rangle|0\rangle & \rightarrow e^{i(\varphi_{01}+\varphi_{10})}|0\rangle|1\rangle \\
|1\rangle|0\rangle & \rightarrow e^{i\varphi_{10}}|0\rangle|1\rangle & \rightarrow e^{i(\varphi_{10}+\varphi_{01})}|1\rangle|0\rangle \\
|1\rangle|1\rangle & \rightarrow e^{i\varphi_{11}}|0\rangle|0\rangle & \rightarrow e^{i(\varphi_{11}+\varphi_{00})}|1\rangle|1\rangle.
\end{align*}
\]

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

\[
\Delta \theta = \delta \theta - \langle \delta \theta \rangle
\]
(as before, ⟨.;⟩ denotes the thermal average), and the gate operator

\[ G \equiv S(RU)^2, \]

where

\[ S \equiv |0⟩⟨0|e^{-2i\xi^2\Phi(\omega)} + |1⟩⟨1|e^{-i[2i\xi^2\Phi(\omega\sqrt{1+e})]-\langle\delta\theta\rangle}}, \]

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

\[ \pi = 4\xi^2 [\Phi(\omega) - \Phi(\omega\sqrt{1+e})] - 2\langle\delta\theta\rangle, \]

we obtain

\[
\begin{align*}
|0⟩|0⟩ & \overset{G}{\longrightarrow} e^{i\Theta}|0⟩|0⟩ \\
|0⟩|1⟩ & \rightarrow e^{-i\Delta\theta_e}\varepsilon^0|0⟩|1⟩ \\
|1⟩|0⟩ & \rightarrow e^{-i\Delta\theta_e}\varepsilon^0|1⟩|0⟩ \\
|1⟩|1⟩ & \rightarrow e^{i\pi}\varepsilon^0|1⟩|1⟩.
\end{align*}
\]

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 \( F^c \) and the quantum fidelity \( F \) is the numerical pre-factor 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 \( \tilde{n} \sim 6 \), 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. (45) that in this case, apart again from an overall phase,

\[
\begin{align*}
|0⟩|0⟩ & \overset{G^g}{\longrightarrow} e^{i\Theta}|0⟩|0⟩ \\
|0⟩|1⟩ & \rightarrow e^{-i\Delta\theta_e}\varepsilon^0|0⟩|1⟩ \\
|1⟩|0⟩ & \rightarrow e^{-i\Delta\theta_e}\varepsilon^0|1⟩|0⟩ \\
|1⟩|1⟩ & \rightarrow (-1)^g|1⟩|1⟩.
\end{align*}
\]

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

\[ F(g)(T) = 1 - g^2[1 - F(T)], \]

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

E. One-dimensional calculation for many ions

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

\[ \bar{r}_j = (x_j, y_j, z_j) = jd \]

in Eq. (10a). Expanding the interaction Hamiltonian \( H_{ij} \), Eq. (10b), in powers of the \( r_i \) and \( r_j \), and neglecting terms of \( o((a_\omega/d)^3) \), we find

\[ H \approx \frac{m\omega^2}{2}\left\{ \sum_{i=1}^{N} \left[ \frac{\omega^2}{\omega^2}(x_i - \bar{x}_j)^2 + y_i^2 + z_i^2 - \varepsilon_i \right. \right. \]

\[ -2a_\omega F(t)|1⟩⟨1|(x_i + \bar{x}_j) \right] + \sum_{i<j}^{N} \frac{x_i x_j}{|i-j|^3} \right\}, \]

where the various quantities are defined in App. B.7. Eq. (50) describes a set of independent forced harmonic oscillators, like the ones we solve in App. 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 App. B.3. We take as initial state

\[ |\Psi_N(t_0)\rangle = \prod_{i=1}^{N} |n_i⟩|\alpha_i⟩_i, \]

where \( \alpha_i \) denotes the internal state of the \( i \)-th ion, and \( n_i \) its motional state in the well corresponding to the \( i \)-th term of the first sum at the right-hand side of Eq. (50). We obtain

\[ |\Psi_N(t)\rangle = \frac{1}{2} \prod_{i=1}^{N} \left( e^{i\phi} \prod_{j \neq i} e^{i\phi_{\alpha_i \alpha_j}} \right) |\Psi_N(t_0)\rangle, \]

where (calculating the two-particle phases \( \phi_{\alpha_i \alpha_j} \) perturbatively)

\[
\begin{align*}
\phi_{\alpha} & \approx \alpha_{i}^{2} ξ^2 \Phi(\omega_i) + \alpha_{i}^{2} \sqrt{\pi} \omega \xi \bar{x}_i / a_\omega \\
& - [n_{x,i} \omega_i + (n_{y,i} + n_{z,i})]\omega(t - t_0), \quad (53a) \\
\phi_{\alpha_i \alpha_j} & \approx \epsilon \int_{t_0}^{t} \langle\Psi_N(t_0)|U_0(t,t')| \frac{x_i x_j}{|i-j|^3} U_0(t',t_0) |\Psi_N(t_0)\rangle dt' \\
& = \sqrt{\frac{\pi}{8}} \frac{\alpha_i \alpha_j}{|i-j|^3} (1 + e\eta_1)(1 + e\eta_2) \\
& \approx \frac{\alpha_i \alpha_j}{|i-j|^3} \theta_d, \quad (53b)
\end{align*}
\]

the last line following from \( \epsilon \ll 1 \) and Eq. (B.40). Again, the result to this order turns out to be independent of the motional state of any of the ions. In the case of two ions, Eq. (53b) gives back Eq. (29).
VI. CONCLUSIONS

We analyzed in detail a recent proposal for scalable quantum computation with ions in an array of microtraps. This scheme bears important advantages over the previous proposal, based on trapped ions as well. Indeed, in that case many ions, lying in a single trap minimum, exchange information via the 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 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 π-pulse), the phase shift is insensitive, to a high accuracy, on the motional state of each ion inside each trap, and therefore the fidelity turns out to be practically independent from 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 μs. 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 really a good candidate for a scalable implementation of a quantum computer.

Acknowledgments

This research has been supported by the Austrian Science Foundation, the Institute for Quantum Information GmbH, and the European Commission through contracts ERB-FMRX-CT96-0087 and HPMF-CT-1999-00211. T.C. acknowledges support from Istituto Trentino di Cultura.

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. ([13a] and [13b]), describing the Hamiltonian Eq. ([1]) for two ions, in the center-of-mass and relative-motion coordinate systems. Indeed the Hamiltonian, with the number of ions N = 2, may be rewritten as \( H = H_R + H_r \), where

\[
H_R = \frac{\mathbf{P}^2}{2M} + \frac{1}{2} M \omega^2 \mathbf{R}^2 - \mathbf{F}(t) \cdot (\mathbf{R} + \mathbf{R}_0) \quad (A1a)
\]

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

and

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

\[
\mathbf{r} \equiv (x, y, z) \equiv \mathbf{r}_2 - \mathbf{r}_1 - \mathbf{d}, \quad (A2b)
\]

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

\[
\mathbf{P} \equiv \mathbf{p}_1 + \mathbf{p}_2, \quad \mathbf{P} \equiv \frac{\mathbf{p}_2 - \mathbf{p}_1}{2}, \quad (A2d)
\]

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

\[
M \equiv 2m, \quad \mu \equiv \frac{m}{2}, \quad \lambda \equiv \frac{q^2}{4\pi\varepsilon_0}. \quad (A2f)
\]

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. (A2d). The correction \( \delta x \equiv d - d_0 \) is the solution of the equation

\[
0 = \frac{\partial}{\partial x} \left( \frac{1}{2} \mu \omega^2 x^2 + \frac{\lambda}{x + d_0} \right) = \mu \omega^2 x - \frac{\lambda}{(x + d_0)^2} \quad (A3)
\]
\[ 
\delta x = \frac{4d_0}{3} \sinh^2 \left\{ \frac{1}{6} \ln \left[ \eta + 1 + \sqrt{\eta(\eta + 2)} \right] \right\}, \quad (A4) 
\]

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

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

where each of the multipole terms \( P_k \) is a polynomial of \( k \)-th degree in \( x, y \) and \( z \) for instance,

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

\[ 
P_4(x, y, z) = x^4 - 3\alpha^2(y^2 + z^2) + \frac{3}{8}(y^2 + z^2)^2. \quad (A6b) \]

By virtue of Eq. (A3), the linear term in the expansion Eq. (A3) cancels exactly with the one arising from the harmonic potential \( \mu \omega^2(r + d - d_0)^2/2 \) in Eq. (A11b). We define the unperturbed Hamiltonians

\[ 
H_R^0 = \frac{P^2}{2M} + \frac{1}{2}M \omega^2 R^2, \quad H^0_s = H_x + H_\perp, \quad (A7) 
\]

where

\[ 
H_x = \frac{p^2}{2\mu} + \frac{1}{2}\mu \omega^2 x^2, \quad (A8a) \]

\[ 
H_\perp \equiv \frac{p_x^2 + p_y^2}{2\mu} + \frac{1}{2}\mu \omega^2 (y^2 + z^2); \quad (A8b) \]

the higher-multipoles contribution

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

the force terms

\[ 
F(t) = \frac{h \omega}{a_\omega} (\hat{\Pi}_1 + \hat{\Pi}_2) \mathcal{F}(t), \quad \mathcal{F}(t) = \frac{h \omega}{a_\omega} \hat{\Pi}_2 - \hat{\Pi}_1 \mathcal{F}(t), \quad (A10) 
\]

where \( \hat{\Pi}_i^\alpha \) is the projector onto the internal state \( \alpha \) of particle \( \iota \):

\[ 
\hat{\Pi}_1 \equiv |1\rangle_1 \langle 1| \otimes 1_2, \quad \hat{\Pi}_2 \equiv 1_1 \otimes |1\rangle_2 \langle 1|. \quad (A11) 
\]

the rescaled frequencies

\[ 
\nu \equiv \omega \sqrt{1 + \epsilon}, \quad \nu_\perp \equiv \omega \sqrt{1 - \epsilon/2}; \quad (A12) 
\]

and the shifted coordinate and energy scales

\[ 
X_0 \equiv R_0 \cdot (1, 0, 0), \quad E_0 \equiv \frac{\lambda}{d} + \frac{1}{2} \mu \omega^2 \delta x^2. \quad (A13) 
\]

Shifting the coordinate system by \( R_0 \sim d \) and the energy scale by \( E_0 \), we finally obtain Eqs. (A3a) and (A3b).

2. Fidelity

The goal of this Section is to show the derivation of the analytical temperature dependence of the fidelity, Eq. (B1). We begin by writing the two-particle phase as

\[ 
\varphi_{cl}^{ab} - \langle \varphi_{cl}^{ab} \rangle = \delta_{ab} \left[ (-1)^a \kappa + 1 \right] \varepsilon + o[(a_\omega/d)^3], \quad (A14) 
\]

where

\[ 
\kappa \equiv \frac{d}{\sqrt{2\varepsilon a_\omega}}, \quad (A15a) \]

\[ 
\varepsilon = \frac{3\theta_{el}}{\hbar \omega} \left( \frac{a_\omega}{d} \right)^2 \left\{ E_1 + E_2 - 2 \sqrt{E_1 E_2} \cos[\omega(t_1 - t_2)] \right\} - 2kB_T \right\}. \quad (A15b) 
\]

We define

\[ 
\Xi(a, b) \equiv |\langle \chi_{cl} | \chi_{cl}(t) \rangle|^2 = 2 \left\{ a \left[ 1 - \cos[(\kappa - 1) \varepsilon] \right] - b \cos[(\kappa - 1) \varepsilon] \right\} \quad (A16) 
\]

\[ 
\times (a + b + 1) + (b - 1)^2 + b [b + 2a \cos(2\kappa \varepsilon)], \quad (A16) 
\]

where \( a \equiv |c_{01}|^2, b \equiv |c_{10}|^2 \), and the normalization of \( |\chi_{cl}\rangle \), in the form \( 1 = \sum_{a, b} |c_{ab}|^2 \), has been taken into account. From Eq. (B1) it follows

\[ 
F_{el} = \min \langle \Xi(a, b) \rangle = \left\langle \min \langle \Xi(a, b) \rangle \right\rangle \quad (A17) 
\]

which is a constrained minimization problem, with constraints 0 \( \leq a \leq 1, \ 0 \leq b \leq 1 \). The solution cannot be found by simply equating the partial derivatives of \( \Xi(a, b) \) to zero, since as it 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

\[ 
\partial_a \Xi(a, b) = -2\varepsilon^2(\kappa - 1)^2 \left( b \frac{\kappa + 1}{\kappa - 1} + \frac{1}{2} - a \right) + o[\varepsilon^3], \quad (A18a) \]

\[ 
\partial_b \Xi(a, b) = -2\varepsilon^2(\kappa + 1)^2 \left( a \frac{\kappa - 1}{\kappa + 1} + \frac{1}{2} - b \right) + o[\varepsilon^3]. \quad (A18b) 
\]

While looking for the minimum, we will neglect \( o[\varepsilon^3] \propto e^{-a_\omega/d} \) – 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

\[ 
b \leq \left( a - \frac{1}{2} \right) \frac{\kappa - 1}{\kappa + 1}, \quad (A19) 
\]

it is \( \partial_b \Xi(a, b) \leq -2\kappa(\kappa + 1) < 0 \). 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
\[ a < b \frac{\kappa + 1}{\kappa - 1} + \frac{1}{2}. \]  
(A20)
The latter, by Eq. (A18b), implies \( \partial_x \Xi(a, b) < 0 \). Summing up, the minimum is reached for the values \((a_0, b_0)\) of the parameters, where
\[ a_0 = 1, \quad \frac{1}{2} \frac{\kappa - 1}{\kappa + 1} < b_0 \leq 1. \]  
(A21)
The problem is therefore reduced to a one-dimensional constrained minimization: We have to study the equation
\[ 0 = \partial_a \Xi(a_0, b) = 2 (\cos(2\kappa \varepsilon) - \cos((\kappa - 1)\varepsilon)) - 2b (\cos((\kappa + 1)\varepsilon) - 1), \]  
(A22)
which has solution
\[ b = \frac{1}{2} \frac{\sin[(3\kappa - 1)\varepsilon/2]}{\sin[(\kappa + 1)\varepsilon/2]} \]  
(A23)
Since the constraint \( b_0 \leq 1 \) has to be fulfilled, we obtain \( b_0 = \min\{b, 1\} \). Indeed, it is \( b \leq 1 \) only for \( \varepsilon \geq f_\kappa(\varepsilon) \), where
\[ f_\kappa(\varepsilon) = 2 \arcsin \left[ \frac{\sin(3\kappa \varepsilon/2) - 2 \sin(\kappa \varepsilon)}{\sqrt{5 + 4 \cos(2\kappa \varepsilon)}} \right]. \]  
(A24)
Hence, to \( \mathcal{O}(\rho_\omega/d)^4 \),
\[ F_{c1} \approx \begin{cases} \frac{1}{2} (1 + \langle \cos[(3\kappa - 1)\varepsilon]\rangle) & \varepsilon \geq f_\kappa(\varepsilon), \\ 1 - 4 \langle \cos(\kappa \varepsilon) \rangle \langle \cos(\varepsilon) - \cos(\kappa \varepsilon) \rangle & \text{otherwise}. \end{cases} \]  
(A25)
Now, we \( f_\kappa'(0) = \kappa/3 > 1 \) (the inequality following from \( \rho_\omega \ll d \)). Hence for small \( T \) such that \( \langle \varepsilon \rangle \ll 1 \), i.e., \( k_B T \ll \hbar \omega (d/\rho_\omega)^2 \), it is \( \varepsilon \ll f_\kappa(\varepsilon) \) and the form of \( F_{c1} \) is given by the second row at right-hand side of Eq. (A25), which we can expand in Taylor series around \( T = 0 \) for taking the thermal average to finally obtain Eq. (B1). When \( \kappa = 0 \), i.e., the third-order anharmonic correction is suppressed,
\[ \Xi(a, b) \bigg|_{\kappa=0} = 1 + 2(a + b - 1)(a + b)[1 - \cos(\varepsilon)]. \]  
(A26)
The function to be minimized depends now only on the sum \( a + b \). Therefore the minimum can be searched 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 \( b \). Eq. (A25) gives the solution also in this case. In particular, since \( f_\kappa=0(\varepsilon) \equiv 0 \leq \varepsilon \forall \varepsilon \), the analytical expression for the fidelity is now given by the first row at right-hand side of Eq. (A25), which for \( \kappa = 0 \) becomes simply
\[ F_{c1}' = F_{c1} \bigg|_{\kappa=0} \approx \frac{1}{2} \left[ 1 + \langle \cos(\varepsilon) \rangle \right]. \]  
(A27)
The same procedure can be used for the minimization over the possible internal states also in the quantum case, as is done in App. B. By expanding Eq. (A27) to lowest nonzero order in powers of \( \rho_\omega/d \), we obtain finally Eq. (B2).

**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 as well 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. (A8). In the ideal case where the external degrees of freedom factorize out at the end of the computation, the evolution operator Eq. (A8) 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
\[ S_j = e^{-i\varphi_j} \sum \alpha \langle \alpha | j \rangle \langle \alpha | e^{i\varphi_j}, \]  
(B1)
where \( \varphi_j \) has to be equal to the kinetic phase acquired after the gate operation by particle \( j \), and we choose
\[ s_1^0 = -\varphi^{00}/2, \quad s_1^1 = -\varphi^{10} + s_0^0; \]
\[ s_2^0 = s_1^0, \quad s_2^1 = -\varphi^{01} + s_1^0. \]  
(B2)
Under these conditions, the compound operator
\[ U(t) \equiv (S_1 \otimes S_2) U(t, t_0) \]  
(B3)
implies the transformation Eq. (B1), with \( \varphi \) given by Eq. (A8).

2. **Unperturbed solution**

As explained in the text, since we assume \( d \gg \rho_\omega \) 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 exactly the unperturbed problem, i.e., we calculate the time-dependent evolution dictated by \( H(t) - H_1 \). So we want to solve the Schrödinger equation
\[ i\hbar \dot{\Psi}(t) = [H_R(t) + H_1^0(t) - f(t) \cdot (r + d)] \Psi(t), \]  
(B4)
with initial condition
\[ |\Psi(t_0)\rangle \equiv |\psi_R(t_0)\rangle_R |\psi_I(t_0)\rangle_I |\alpha\rangle_1 |\beta\rangle_2. \]  
(B5)
The subscript $R$ ($r$) denotes the center-of-mass (relative) motion, as defined in App. A.1. The solution is

$$
|\psi_R(t)\rangle_R = e^{-iH_0^r(t-t_0)/\hbar} e^{iX_0^r\int_{t_0}^t F(t')dt'/\hbar}
$$

$$
\times \exp \left[-\int_{t_0}^t ds K_R(s,t_0) \frac{dK_R^*(s,t_0)}{ds}\right]
\times e^{-iK_R(t,t_0)\hat{a}_R^\dagger e^{-iK_R^*(t,t_0)\hat{a}_R} \left|\psi_R(t_0)\right\rangle_R},
$$
(B6a)

$$
|\psi_r(t)\rangle_r = e^{-iH_0^r(t-t_0)/\hbar} e^{i\phi^r f(t')dt'/\hbar}
$$

$$
\times \exp \left[-\int_{t_0}^t ds K_r(s,t_0) \frac{dK_r^*(s,t_0)}{ds}\right]
\times e^{-iK_r(t,t_0)\hat{a}_r^\dagger e^{-iK_r^*(t,t_0)\hat{a}_r} \left|\psi_r(t_0)\right\rangle_r},
$$
(B6b)

where $\hat{a}_R$ ($\hat{a}_r$) is the annihilation operator for the $x$ component of the center-of-mass (relative) motion, and

$$
K_R(t,t_0) = \frac{1}{\sqrt{2\mu \omega}} \int_{t_0}^t dt' F(t') e^{i\omega (t'-t_0)} ,
$$
(B7a)

$$
K_r(t,t_0) = \frac{1}{\sqrt{2\mu \nu'}} \int_{t_0}^t dt' \frac{F(t')}{E(t')},
$$
(B7b)

Now the explicit form of the force term, Eq. (B2), can be inserted into Eqs. (B7a) and (B7b) through Eq. (A13), to yield

$$
K_R(t,t_0) = \left[\Pi_1 + \Pi_2\right] K (\omega, t, t_0) ,
$$
(B8a)

$$
K_r(t,t_0) = \left[\Pi_2 - \Pi_1\right] K (\nu, t, t_0) ,
$$
(B8b)

where

$$
K (\omega, t, t_0) = \frac{\sqrt{\pi}}{4} \omega \tau e^{-(\omega\tau/2)^2} I (\omega, t')^{t}_{t_0},
$$
(B9a)

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

We take as initial state

$$
|\psi_R(t_0)\rangle_R \equiv |N\rangle_R \equiv |N_x\rangle_X|N_y\rangle_Y|N_z\rangle_Z ,
$$
(B10a)

$$
|\psi_r(t_0)\rangle_r \equiv |n\rangle_r \equiv |n_x\rangle_x|n_y\rangle_y|n_z\rangle_z .
$$
(B10b)

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

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

which turns out to be given by

$$
\phi_{_{\alpha}\beta} = \phi_{R_{_{\alpha}\beta}} + \phi_{r_{_{\beta}}},
$$
(B12a)

$$
\phi_{R_{_{\alpha}\beta}} \approx (\alpha + \beta)^2 \xi^2 \Phi (\omega) + (\alpha + \beta) \sqrt{\pi} \omega \xi X_0 / a_\omega,
$$
(B12b)

$$
- (N_X + N_Y + N_Z) \omega (t - t_0),
$$

$$
\phi_{r_{_{\beta}}} \approx (\alpha - \beta)^2 \xi^2 \Phi (\nu) - (\alpha - \beta) \sqrt{\pi} \omega \xi X_0 / a_\omega,
$$
(B12c)

$$
- [n_x \nu + n_y \nu + n_z \nu_z] (t - t_0),
$$

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

with

$$
A \equiv \Im [I (\omega, t_0)] - i P (\omega, 0),
$$

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

$$
C \equiv 2 \sqrt{A^2 (\omega^2 / 2 + 1/\tau^2) - A \sqrt{\pi} e^{(\omega\tau/2)^2} / 4},
$$

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

$$
O^{(n)} (t, t_0) \equiv |\langle \Psi(t) | \Psi(t_0) \rangle| = O^{(n)}_{R} O^{(n)}_{r},
$$
(B14)

where

$$
O^{(n)}_{R} = M (-N_X, 1, |K_R(t,t_0)|^2) e^{-\frac{i}{2} |K_R(t,t_0)|^2},
$$
(B15a)

$$
O^{(n)}_{r} = M (-n_x, 1, |K_r(t,t_0)|^2) e^{-\frac{i}{2} |K_r(t,t_0)|^2},
$$
(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

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

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

$$
U_j (t, t_0) \equiv \frac{1}{(i\hbar)^j} \int_{t_0}^{t} dt_j \int_{t_0}^{t_j} dt_{j-1} \ldots \int_{t_0}^{t_{j-2}} dt_{j-2} \int_{t_0}^{t_{j-1}} dt_1 U_0 (t, t_j)
$$

$$
\times H_1 U_0 (t_j, t_{j-1}) H_1 U_0 (t_{j-1}, t_{j-2}) \ldots \times U_0 (t_2, t_1) H_1 U_0 (t_1, t_0).
$$
(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. (B11). Since $\langle U_0 (t, t_0) \rangle$ is given by Eq. (B11), we just need to compute

$$
\langle U_1 (t, t_0) \rangle \equiv \frac{1}{i\hbar} \int_{t_0}^{t} dt' O^{(1)} (t, t', t_0) e^{i\phi^1(t, t') + \phi^{0\beta}(t, t_0)}
$$

$$
= \frac{e^{i\phi^1(t, t_0)}}{i\hbar} \int_{t_0}^{t} dt' O^{(1)} (t, t', t_0) ,
$$
(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

$$ O_{\alpha}^{\beta}(t', t, t_0) \equiv \langle \psi(t) | U_0(t, t') H_1 U_0(t', t_0) | \psi(t_0) \rangle. \tag{B19} $$

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 Sect. V 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 wavefunction of the evolved state is then

$$ |\langle \psi_{x}(t_0) | U_0(t, t_0) | x \rangle | \approx |\langle \rho | U_0(t', t_0) | \psi_{x}(t_0) \rangle| \approx \psi_x(x - f(t)/\mu \nu^2) \psi_y(y) \psi_z(z), $$

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

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

where

$$ \Delta^{\alpha\beta} \equiv - \frac{\sqrt{\pi} \lambda}{\hbar d} \sum_{k=3}^{\infty} \frac{a_{\nu} \xi}{d} \delta_k, \tag{B22a} $$

$$ \Delta' \equiv - \frac{t-t_0}{\hbar d} \sum_{k=3}^{\infty} \frac{a_{\nu} \xi}{d} \delta'_k, \tag{B22b} $$

$$ \delta_k \equiv \frac{1}{\sqrt{\pi} \sigma_{x}} \int_{t_0}^{t} d't' (\mathbf{n} \cdot \mathbf{P} \cdot \mathbf{F}) | P_k (x + \frac{\omega^2}{\nu^2} a_{\omega} (t', y, z) - P_k (x, y, z) | \mathbf{n} \rangle, \tag{B22c} $$

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

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

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. (B21), given that $|\Delta^{\alpha\beta} + \Delta'| = |\Delta_1(t_0, t)\rangle \ll |\langle U_0(t, t_0) \rangle| \approx 1$. The internal-state-independent part $\Delta'$ cancels out when computing the gate phase Eq. (B2), 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 depend neither on the internal state nor 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 $|\mathbf{n}\rangle$ of $H_{\nu}^0$, as is done in Eq. (B22d), but rather those of the full Hamiltonian $H_\nu$. However, as we will demonstrate in the next Section, the corrections are of $O(\langle a_{\omega}/d\rangle^3)$ and therefore we will consistently not take them into account in the present calculation. The relevant matrix elements are

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

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

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

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

Hence

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

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

$$ \delta'_3 = 0, \tag{B25c} $$

$$ \delta'_4 = \frac{3}{4} [2n_x(n_x + 1) + 1] - \frac{3}{2} \nu(2n_x + 1)(n_y + n_z + 1) + \frac{3}{16} \nu^2 [n_y(3n_y + 5) + n_z(n_z + 5) + 4(1 + n_y n_z)] \tag{B25d} $$

where $\nu = \nu / \nu_\perp$.

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

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

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

$$ H_\nu^1 \equiv \frac{\hbar \omega d^2}{2 a_{\omega}^2} \sum_{k=3}^{\infty} P_k (x, y, z) \frac{d^k}{d^k}. \tag{B27} $$
Therefore we make a perturbative expansion in the small parameter $\epsilon$. So we write the eigenstates of $H_\tau$ (omitting throughout this Section the subscript $r$) as

$$|n(\epsilon)\rangle = \sum_{i=0}^{\infty} \epsilon^i |n^{(i)}\rangle,$$  \hspace{1cm} (B28)

where the first terms are

$$|n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle m^{(0)} | H_1 \rangle |n^{(0)}\rangle}{E^{(0)}_m - E^{(0)}_n} |m^{(0)}\rangle,$$  \hspace{1cm} (B29a)

$$|n^{(2)}\rangle = \sum_{l \neq m} \frac{\langle m^{(0)} | H_2^e \rangle |l^{(0)}\rangle |l^{(0)} | H_1 \rangle |n^{(0)}\rangle}{(E^{(0)}_m - E^{(0)}_n)} |m^{(0)}\rangle,$$  \hspace{1cm} (B29b)

and $|n^{(0)}\rangle$ are the eigenstates of $H_0^e$, with eigenenergies $E^{(0)}_n$. The $k^{th}$ term in $H_1$ gives a contribution of order $\sim (h\omega/2)(a_\omega/d)^{k-2}$. Since we want to neglect corrections of order $o((a_\omega/d)^{k})$, we need to go up to $k = 4$ in the expansion of $H_1^e$. But from Eqs. (A6a) and (A6b) it is straightforward to see that $\langle m^{(0)} | P_{3,4}(x,y,z) |n^{(0)}\rangle$ for $m \neq n$. It follows that

$$|n(\epsilon)\rangle = |n^{(0)}\rangle + o((a_\omega/d)^{k}),$$  \hspace{1cm} (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 $H_0^e$.

5. Numerical computation

The goal of this Section is to transform the Schrödinger equation for the two-particle wavefunction 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 wavefunction (omitting for simplicity the subscript $r$) as

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

$$\dot{c}_{nl} = \frac{i}{\hbar} \sum_{n',l'=0}^{\infty} c_{n'l'}(t) e^{i[(n-n')\nu + (l-l')\nu_\perp]t} \times \langle nl | f(t) x - H_1 | n'l' \rangle$$

$$= \frac{i}{\hbar} \left[ \frac{\partial}{\partial \nu} \left( \sqrt{n} e^{i\nu t} c_{n-1,l} + \sqrt{n+1} e^{-i\nu t} c_{n+1,l} \right) \right]$$

$$+ \lambda \int \sum_{k=3}^{\infty} \left( \frac{\partial}{\partial \nu} \right)^k \left( c^{(k)}_{nl} \right),$$  \hspace{1cm} (B32)

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

$$C^{(3)}_{nl} = \sqrt{n(n-1)(n-2)} e^{3i\nu t} c_{n-3,l}$$
$$+ 3n^{3/2} e^{i\nu t} c_{n-1,l} + (n+1)^{3/2} e^{-i\nu t} c_{n+1,l}$$
$$+ \sqrt{n(n+1)(n+2)} e^{2i\nu t} c_{n-2,l}$$
$$+ 2(n+1) \left( c^{(2)}_{nl} \right)$$

$$\left( + (n+1)(n+2) e^{2i\nu t} \right) c_{n-1,l}$$
$$+ (n+2)(n+1) e^{i\nu t} c_{n+1,l} + 2(n+1) c_{n-1,l} + 2(n-1) c_{n+1,l} \right\};$$

$$C^{(4)}_{nl} = -\sqrt{n(n-1)(n-2)} \left( n-3 \right) e^{4i\nu t} c_{n-4,l}$$
$$+ \sqrt{n(n-1)} e^{2i\nu t} \left\{ 3\tilde{\nu} \left[ \sqrt{(n-1)(n-2)} e^{2i\nu t} c_{n-2,l} \right]$$
$$+ \sqrt{(n+1)(n+2)} e^{-2i\nu t} c_{n-1,l}$$
$$+ (2(n+1)) c_{n-2,l} \right] - 2(n-2) c_{n-1,l} \right\}$$

$$- \frac{3\tilde{\nu}^2}{8} \sqrt{(n-1)(n-2)(n-3)} e^{4i\nu t} c_{n-4,l} - 3\tilde{\nu} \sqrt{(n-1)(2n-1)} e^{2i\nu t} c_{n-2,l}$$
$$- \left\{ \frac{9\tilde{\nu}^2}{8} \left[ 2(n+1) + 1 \right] - 3\tilde{\nu} (2n+1)(2n+1)$$
$$+ 3 [2(n+1)+1] e^{-2i\nu t} \right\}$$

$$- \frac{3\tilde{\nu}^2}{8} \sqrt{(n+1)(n+2)(n+3)(n+4)} e^{-4i\nu t} c_{n,l+4}$$
$$+ \sqrt{(n+1)(n+2)} e^{-2i\nu t} \left\{ 3\tilde{\nu} \left[ (2n+1)c_{n+2,l} \right]$$
$$+ \sqrt{(l+1)(l+2)} e^{2i\nu t} c_{n+4,l+2}$$
$$+ \sqrt{(l-1)(l+2)} e^{2i\nu t} c_{n+2,l-2} - 2(2n+3) c_{n+2,l} \right\}$$
$$- \sqrt{(n+1)(n+2)(n+3)(n+4)} e^{-4i\nu t} c_{n+4,l}.$$

Excitations higher than a certain level should be absent as long as we are in an adiabatic regime. Thus in
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 Θ appearing in Eq. (45) can be computed from Eqs. (B12a)-(B12d) and (B22a)-(B22d), as

\[ \Theta \approx 2\omega \left\{ \sqrt{\pi \xi \tau \frac{X_0}{a_\omega} - \left[ \sum_{i=1}^{6} n_i + \epsilon \sum_{k=3}^{\infty} \left( \frac{a_\omega}{d} \right)^{\delta_k^i} (t - t_0) \right] \right\}, \]

(B34)

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

\[ |\chi'\rangle = \sum_{\alpha, \beta = 0}^{1} (-1)^{\alpha \beta} c_{\alpha \beta} |\alpha'\rangle \otimes |\beta\rangle. \]

(B35)

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

\[ \sigma_T = \rho_T(t_0) \otimes |\chi\rangle \langle \chi|, \]

(B36)

where \( \rho_T(t_0) \) is defined in Eq. (B33), and we recall that \( \omega \approx \nu \approx \nu_\perp \). After the gate operation we have

\[ \sigma'_T = \sum_{\alpha, \beta, \alpha', \beta'} c_{\alpha \beta} c_{\alpha' \beta'} G_{\alpha \beta} \rho_T(t_0) G_{\alpha' \beta'}^† |\alpha'\rangle \otimes |\beta\rangle \langle \beta|, \]

(B37)

where \( G_{\alpha \beta} \equiv \langle \alpha | \beta \rangle |\alpha\rangle \langle \beta| \), and the gate operator \( G \) is defined in Eq. (15). As already stated in Sect. V A, because of adiabaticity, the motional state after the gate operation is unchanged, i.e. \( G_{\alpha \beta} \rho_T(t_0) G_{\alpha' \beta'}^† \approx \rho_T(t_0) \). If \( \theta = \pi \), the minimum fidelity \( F(T) \), given by Eq. (5), is

\[
F(T) = \min_{\{c_{\alpha \beta}\}} (1 - \gamma)^6 \prod_{i=1}^{6} \sum_{n_i=1}^{\infty} \gamma^{n_i} (n_i) \left[ (|c_{00}|^2 + |c_{11}|^2)^2 \right. \\
+ 2 (|c_{00}|^2 + |c_{11}|^2) (|c_{01}|^2 + |c_{10}|^2) \cos(\Delta \theta) \\
+ (|c_{01}|^2 + |c_{10}|^2)^2 \left. |n_i| \right] \\
= \frac{(1 - \gamma)^3}{2} \prod_{i=1}^{3} \sum_{n_i=1}^{\infty} \gamma^{n_i} (n_i) [1 + \cos(\Delta \theta)] |n_i| (B38)
\]

\[
\approx 1 - \frac{6^3 \theta_{cl}^2}{(1 + e^5)(1 - e^{-2}/4)} \left( \frac{a_\omega}{d} \right)^4 \frac{e^{-\hbar \omega/k_B T}}{(1 - e^{-\hbar \omega/k_B T})^2}
\]

where the minimization over the coefficients \( \{c_{\alpha \beta}\} \) has been carried out exactly as in App. 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. (10) follows, by taking into account that \( \epsilon \ll 1 \) and \( \theta_{cl} \approx \theta = \pi \), and expanding in a Taylor series for \( \hbar \omega \ll k_B T \).

7. Many-ions calculation

In this Section we simply give the definitions of the parameters appearing in Eq. (3):

\[
\epsilon_i = \frac{\omega_i^2}{2} x_i^2 - \frac{\epsilon}{2} d^2 \mathcal{H}_{n-i}, \quad \omega_i = \omega \sqrt{1 + \epsilon_i}, \quad \hat{x}_i = \frac{d}{2} \frac{\epsilon_i}{1 + \epsilon_i}, \quad \eta_i = \frac{1}{2} \sum_{j=1}^{N} \frac{1 - \delta_{ij}}{|i - j|^3}
\]

(B39a)

\[
\eta_i' = \frac{1}{2} \sum_{j=1}^{N} \frac{i - j}{|i - j|^3}
\]

(B39b)

\[
\mathcal{H}_k = \frac{1}{2} \left[ \psi^{(2)}(i) + \psi^{(2)}(N + 1 - i) + \zeta(3) \right], \quad \zeta(s) \text{ is the Riemann zeta function. It is}
\]

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