Coherent and optimal control of adiabatic motion of ions in a trap

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Small anharmonicity, created along the axial direction of the trap, allows controlling the motional states of ions adiabatically using electric fields. In this paper several important aspects of this control scheme are explored theoretically. The pulses for various state transformations, including universal quantum gates, are derived using the optimal control theory. They exhibit simple shapes and other favorable properties, which indicate a promising route for practical implementation.

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I. INTRODUCTION

A concept of the ion-trap quantum computer was proposed by Cirac and Zoller in 1995 [1] and implemented experimentally in the same year by Wineland and co-workers [2]. The quantized motional states of a string of ions, combined with electronic states of individual ions, can be used to encode qubits and to practically realize the quantum gates. This field has been very active and a number of the trap architectures and the quantum control scenarios have been proposed and implemented [3–8].

Usually, the trapping potential in the experiment is harmonic and the motional states of ions in the trap are energetically equidistant, analogous to the spectrum of a multidimensional harmonic oscillator. In such an experimental setup the coherent control of ionic motion in the trap can be achieved only through electronic excitation of individual ions into a gateway state and by dumping the population of that state onto other motional states of the ground electronic state. This scheme is carried out routinely using lasers [1–8]. In this paper we theoretically explore an alternative approach. We propose to create some (small) anharmonicity in the trapping potential which would modify the spectrum and allow addressing the motional state-to-state transitions selectively using the microwave electric fields of appropriate frequency, amplitude, duration, and phase. In this scheme all ions remain in the ground electronic state and the motion of ions in the trap is controlled adiabatically. Nowadays the ion trapping techniques undergo revolutionary changes and multiple ion traps are placed on a single microchip [9–11]. Some control tasks can be carried out using the electric fields instead of lasers, which could facilitate the ongoing miniaturization and the practical implementation of scalability in the future.

Note that this control scheme can be used not only to carry out the simplest state manipulations adiabatically (like state flips $|0\rangle \rightarrow |1\rangle$ and $|1\rangle \rightarrow |0\rangle$) but also for more involved transformations like, for example, "cooling" of a superposition state onto the ground motional state: $a|0\rangle + b|1\rangle + c|2\rangle + \cdots \rightarrow |0\rangle$. Also demonstrated here is that it should be feasible to employ this method for applying the quantum logics gates. The qubit states can be traditionally the two lowest motional states $|0\rangle$ and $|1\rangle$ but other choices are equally possible. Moreover, creating anharmonicity in a trapping potential should permit one to employ not just two qubit states, but a progression of several motional states (e.g., $|0\rangle$,$|1\rangle$,$|2\rangle$, $|3\rangle$,…) for the quantum information processing, which may allow executing simple quantum algorithms using a single trapped ion.

II. THEORETICAL FRAMEWORK

In this paper we explore the basic properties of such an adiabatic control scheme using the simplest theoretical model for one ion in a trap where the motion along the trap (z axis) is sufficiently uncoupled from the radial motion, so that the problem is essentially one dimensional. We assume that it is possible to create a small anharmonicity of the trapping potential along the axial direction z, which leads to a nonequidistant (anharmonic) spectrum of the motional states. Such a spectrum can be represented analytically using the standard Dunham expansion formula:

$$E_\nu = \omega_z \hbar \left(\nu + \frac{1}{2} \right) - \Delta_z \hbar \left(\nu + \frac{1}{2} \right)^2, \tag{1}$$

where ω_z is the harmonic frequency and Δ_z is the anharmonicity parameter. The spectrum of Eq. (1) represents eigenvalues of the time-independent Schrödinger equation for the axial direction of the ion trap: $\hat{H}_0 \psi_\nu(z) = E_\nu \psi_\nu(z)$, where

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V_a(z)q$$

is a one-dimensional (1D) Hamiltonian and $V_a(z)$ is the anharmonic trapping potential. In order to control motion of the ion we propose to apply an additional time-dependent electric field $E(z,t)$ along the axis of the trap, so that the Hamiltonian becomes $\hat{H} = \hat{H}_0 + \phi(z,t)q$, where q is the electric charge of the ion and

$$\phi(z,t) = -\int_0^z E(z,t)dz$$

is the electric potential. The easiest approach is to create a spatially homogeneous field with the time-dependent amplitude $E(t)$, which gives

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$$\hat{H} = \hat{H}_0 - E(t)zq. \quad (2)$$

The last term in Eq. (2) can be viewed as the electrostatic energy in the linear potential with the slope $E(t)$ that changes in time. The dependence $E(t)$ defines what we will call *the control pulse*. In the simplest control scenario one can consider, for example, the field amplitude, the pulse duration, and the frequency as control parameters and try to tune them to achieve the desired control, but we go beyond that and search for an optimal pulse shape by allowing $E(t)$ to be a general function of time defined on a grid of time intervals.

In order to design theoretically the pulse shape $E(t)$ for a transfer of the entire population from a given initial state φ_i to a chosen final state φ_f (which can be eigenstates or superposition states) we use the monotonically convergent numerical algorithm of Rabitz [12] where the optimization is achieved by maximizing the objective functional:

$$J_{fi} = |\langle \psi_i(T)|\varphi_f\rangle|^2 - \int_0^T \alpha(t)|E(t)|^2 dt - 2\,\mathrm{Re}\left\{\langle \psi_i(T)|\varphi\rangle \int_0^T \langle \psi_f(t)|\frac{i}{\hbar}\hat{H} + \frac{\partial}{\partial t}|\psi_i(t)\rangle dt\right\}. \quad (3)$$

Here T is the specified pulse duration, $\psi_i(t)$ is the time-dependent wave function driven by $E(t)$, and $\psi_f(t)$ is the wave function driven backward in time. The first term in Eq. (3) represents an overlap of the final wave function with the target state; the second term is required to minimize energy of the pulse and constrain its smooth switching on and off; the last term ensures that evolution of the wave functions $\psi_i(t)$ and $\psi_f(t)$ satisfies the time-dependent Schrödinger equation. Variations of $\delta\psi_i$, $\delta\psi_f$, and δE lead to a set of two time-dependent Schrödinger equations for $\psi_i(t)$ and $\psi_f(t)$ to be propagated forward and backward in time (using φ_i and φ_f as boundary conditions) and the third equation,

$$E(t) = -\frac{qs(t)}{\hbar\alpha_0}\,\mathrm{Im}\langle \psi_i(t)|\psi_f(t)\rangle\langle \psi_f(t)|z|\psi_i(t)\rangle, \quad (4)$$

which permits one to determine the optimal field $E(t)$ iteratively. In Eq. (4) the standard form of the penalty function is used, $\alpha(t)=\alpha_0/s(t)$, where α_0 represents the constant penalty factor and $s(t)$ is a smooth switching function.

It is instructive to compare this problem with the problem of coherent control of molecular vibrations using ultrafast optimally shaped laser pulses [12–17]. There, the semiclassical molecule-light interaction is given by $\hat{H}=\hat{H}_{\mathrm{mol}}-\varepsilon(t)\mu(r)$, where $\hat{H}_{\mathrm{mol}}$ is the molecular Hamiltonian, $\varepsilon(t)$ is the intensity of the time-dependent laser field, and $\mu(r)$ is the molecular dipole moment function. For the nonpolar molecules executing the low amplitude vibrational motion the dipole moment is a linear function of the internuclear distance:

$$\mu(r) \approx \left(\frac{\partial\mu}{\partial r}\right)_{r=r_{\mathrm{eq}}} r + \cdots$$

, so that the total Hamiltonian becomes $\hat{H}=\hat{H}_{\mathrm{mol}}-\varepsilon(t)r\mu'_{r_{\mathrm{eq}}}$. Since this expression is mathematically equivalent to Eq. (2), the optimal control theory methods developed for molecular vibrations can be utilized to control the motion of ions in a trap. However, the computational aspect of this problem is complicated by several special properties of the trapped ions: (i) The spatial extent of the motional wave functions $\psi(z)$ of ions in a trap is $\sim$50 nm, which is 500 times larger than the amplitude of a typical molecular vibration. (ii) The energy differences between the motional states of ions in a trap are $\sim$1 MHz, which is about 10^7 times smaller than in the molecules. (iii) The time scale of ionic motion (and control) is 10^8 times longer than the femtosecond scale of molecular motion. Due to these features the time step for numerical propagation of ionic wave functions was very large, $dt=5$ ns. In order to reduce the field amplitude to the optimal level, the penalty factor we chose had to be very large as well, $\alpha_0=10^{12}$. The overall convergence of iterations was very slow and $\sim 10^4$ forward-backward propagation cycles were necessary to converge $E(t)$.

III. RESULTS AND DISCUSSION

As a prototype, we took the experimental setup used recently by the Monroe group to trap the $^{111}Cd^+$ ions, where the axial frequency is $\omega_z/2\pi=2.77$ MHz [18–20]. It seems possible to create small anharmonicity along the axis of the trap using additional electrodes. Here we began with anharmonicity parameter $\Delta_z/2\pi=27.7$ kHz, which is only 1% of the frequency value. The pulse duration is also somewhat arbitrary and we began by choosing $T=10$ μs. (Below we will explore the range of Δ_z and T values.) As a simple test of feasibility of this approach, we tried to optimize the shape $E(t)$ of the control pulse for the state flips $|0\rangle\rightarrow|1\rangle$ and $|1\rangle\rightarrow|0\rangle$, and also for the simplest example of "cooling:" $\frac{1}{\sqrt{2}}|0\rangle+\frac{1}{\sqrt{2}}|1\rangle\rightarrow|0\rangle$. The optimal pulses derived for these transformations came out simple-shaped and very accurate (able to achieve the probability transfer up to $|\langle \psi_i(T)|\varphi_f\rangle|^2\sim 0.9999$). The frequency spectrum of such pulses exhibits only one peak centered precisely at $\omega_{0\leftrightarrow 1}$. The maximum amplitude of the ac field $E(t)$ is in the range 1.5–2.5 mV/cm. It seems to be relatively easy to create such control pulses in the experiment, and this is the first important conclusion of this paper.

As a more advanced task, we carried out optimization of the pulse for the gate NOT using a multitarget version [13–15] of the objective functional (3). Figure 1(a) shows the optimized shape $E(t)$, while Figs. 1(b) and 1(c) show how the population of the motional states $|0\rangle$, $|1\rangle$, and $|2\rangle$ changes as a function of time during the NOT$|0\rangle\rightarrow|1\rangle$ and NOT$|1\rangle\rightarrow|0\rangle$ transformations. Note that the gate transformation in Fig. 1 is very accurate and the population of states created by the optimal pulse is almost entirely restricted to the qubit states $|0\rangle$ and $|1\rangle$, with only a tiny temporary population in the state $|2\rangle$ and a negligible population in the upper motional states. The shape of the pulse in Fig. 1(a) is simple and is a reflection of the penalty function used in the calculations, $s(t)=\sin^2(\pi t/T)$. Practical realization of such control pulses is relatively straightforward.

In order to demonstrate the effect of anharmonicity we varied the value of the anharmonicity parameter $\Delta_z/2\pi$ in

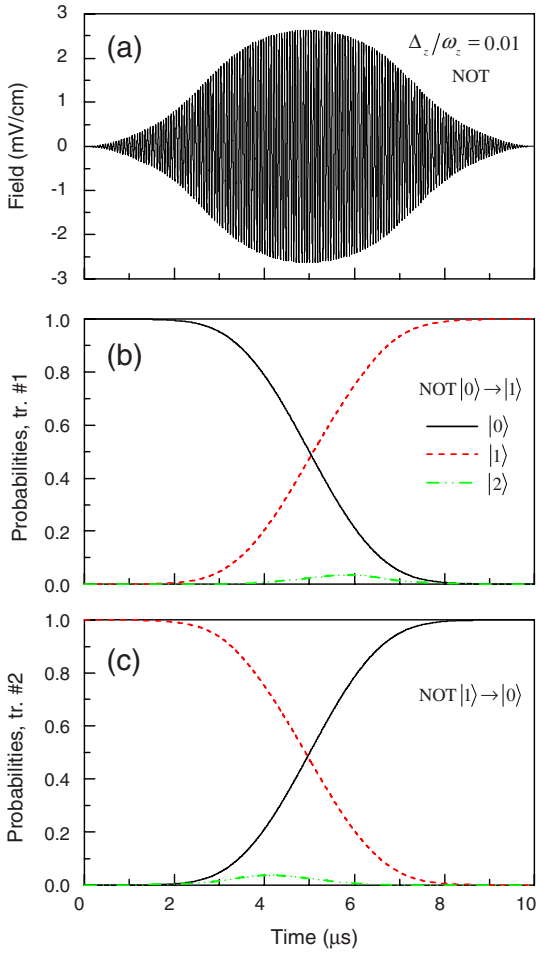

FIG. 1. (Color online) The gate NOT in the Cd^+ ion trap with $\omega_z/2\pi=2.77$ MHz and the anharmonicity parameter $\Delta_z/2\pi=27.7$ kHz: (a) optimally shaped electric field; (b) switching of population between the qubit states during the NOT$|0\rangle \rightarrow |1\rangle$ transformation; (c) the same during the NOT$|1\rangle \rightarrow |0\rangle$ transformation.

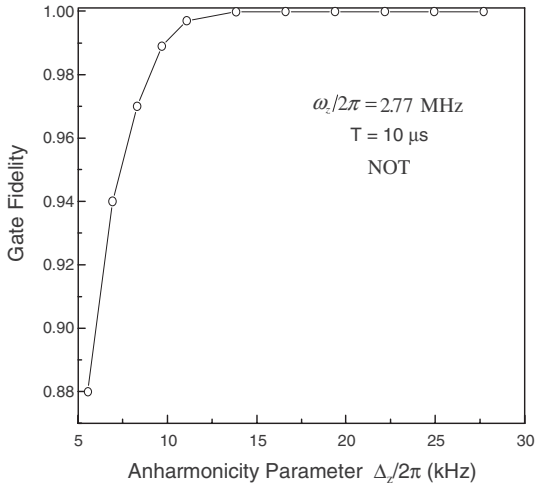

FIG. 2. Fidelity of the gate NOT as a function of anharmonicity parameter for the Cd^+ ion trap with $\omega_z/2\pi=2.77$ MHz. The target time is $T=10$ μs.

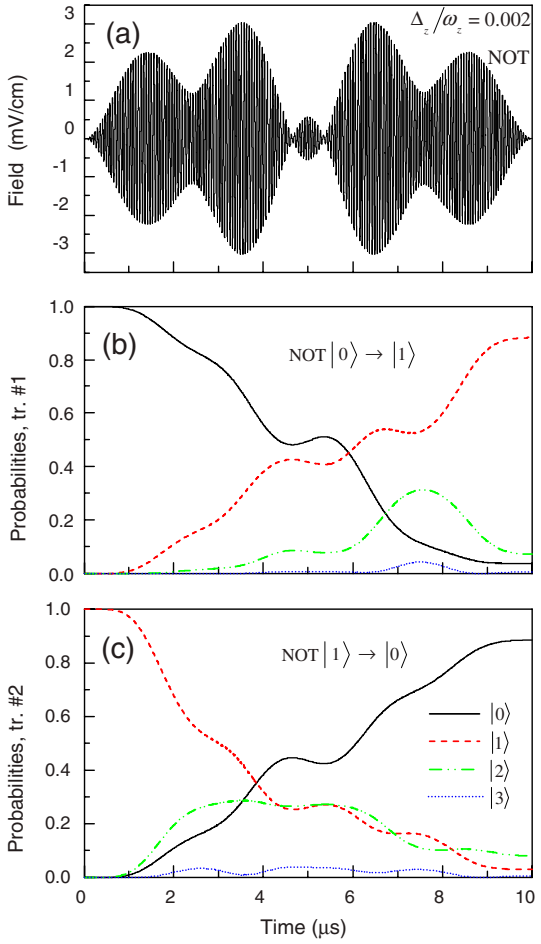

FIG. 3. (Color online) Same as in Fig. 1 but for $\Delta_z/2\pi=5.54$ kHz (an insufficient anharmonicity case).

the range from 5.54 to 27.7 kHz (i.e., between 0.2% and 1% of the frequency value) keeping the values of ω_z and T fixed. For each value of Δ_z we carried out the pulse optimization for the gate NOT and calculated its fidelity $F=\frac{1}{2}\Sigma|\langle\psi_i(T)|\varphi_f\rangle|^2$, where the sum is over the two transitions optimized simultaneously, NOT$|0\rangle \rightarrow |1\rangle$ and NOT$|1\rangle \rightarrow |0\rangle$ [13–15]. The results are summarized in Fig. 2 which shows that the gate fidelity decreases rapidly when the value of $\Delta_z/2\pi$ is reduced to below ~13 kHz. At $\Delta_z/2\pi=5.54$ kHz fidelity drops to $F\approx 0.88$.

More insight into this effect is obtained from analysis of Figure 3, which gives the same information as Fig. 1, except for the weakest anharmonicity considered here ($\Delta_z/2\pi=5.54$ kHz, the worst case in Fig. 2), when it becomes evident that the low fidelity is due to the population transfer to the excited motional states $|2\rangle$ and $|3\rangle$. Not only do these states interfere during the pulse, they also keep some residual population at the final time T. The frequency spectrum of the pulse in Fig. 3 shows several peaks in the range of $|0\rangle \leftrightarrow |1\rangle$, $|1\rangle \leftrightarrow |2\rangle$, $|2\rangle \leftrightarrow |3\rangle$, and $|3\rangle \leftrightarrow |4\rangle$ transition frequencies with the main peak slightly blueshifted from the $\omega_{0\leftrightarrow 1}$ value. Even though the pulse shape in Fig. 3 is more complicated (compared to that of Fig. 1), we still cannot suppress the population of the upper states completely. We monitored the popu-

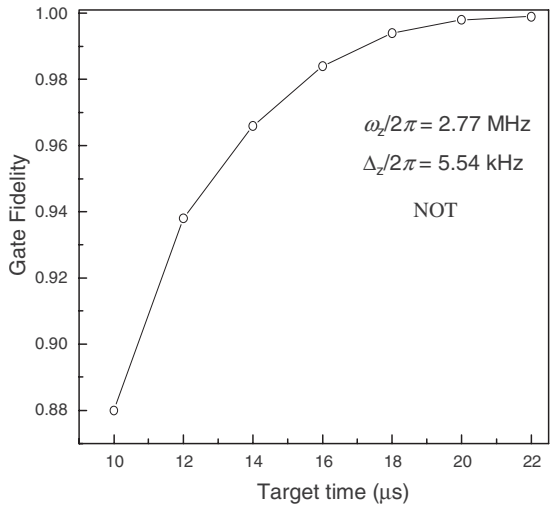

FIG. 4. Fidelity of the gate NOT as a function of pulse duration T for the anharmonicity parameter $\Delta_z/2\pi=5.54$ kHz.

lation of upper motional states during the pulses obtained for different values of Δ_z and found that the maximum probability in the states $|2\rangle$, $|3\rangle$, and $|4\rangle$ decreases from 0.31, 0.043, and 0.002 at $\Delta_z/2\pi=5.54$ kHz to 0.17, 0.006, and 7.5×10^{-5} at $\Delta_z/2\pi=11.08$ kHz, and to only 0.08, 0.001, and 6.0×10^{-6} at $\Delta_z/2\pi=19.39$ kHz. The general idea behind this phenomenon is that when the value of Δ_z is small we approach the limit of a harmonic oscillator, in which several state-to-state transitions interfere and the system is hard to control. In contrast, when the value of Δ_z is large we approach the two-state system limit where the control is very simple. In practice, the value of Δ_z from the high fidelity plateau (see Fig. 1) should give us a reliable controllable system.

In order to demonstrate the effect of the pulse duration T we took the least accurate case from Fig. 2 (i.e., the smallest anharmonicity parameter, $\Delta_z/2\pi=5.54$ kHz) and tried to increase the target time T, keeping the values of ω_z and Δ_z constant. As before, for each set of parameters we optimized the pulse for the gate NOT and calculated its fidelity. The results are presented in Fig. 4 which shows that increasing T allows improving the fidelity steadily and significantly. Using $T=22$ μs we achieved $F\sim0.999$ for the gate NOT. We compared pulses optimized at different values of T and found that when the pulse duration increases, the amplitude of the control field $E(t)$ smoothly decreases. For example, the maximum value of the field was $E_{\max}=3.03$, 2.78, 1.88, and 1.38 mV/cm in the pulses optimized for $T=10$, 12, 14, and 16 μs, respectively. Thus longer pulse duration permits one to use the field of smaller amplitude, which in turn reduces the excitation of upper (interfering) states, simplifies control, and improves accuracy of transformations. It is also clear that longer pulses provide better frequency resolution. Using the uncertainty principle and the spectrum of Eq. (1) it is easy to obtain a relationship between the anharmonicity parameter and the required pulse duration, $T\sim\pi/\Delta_z$, which helps us to understand qualitatively the numerical results given in Figs. 2 and 4.

Finally, for an intermediate value of anharmonicity, $\Delta_z/2\pi=15.5$ kHz (0.6% of $\omega_z/2\pi$), we optimized pulses for

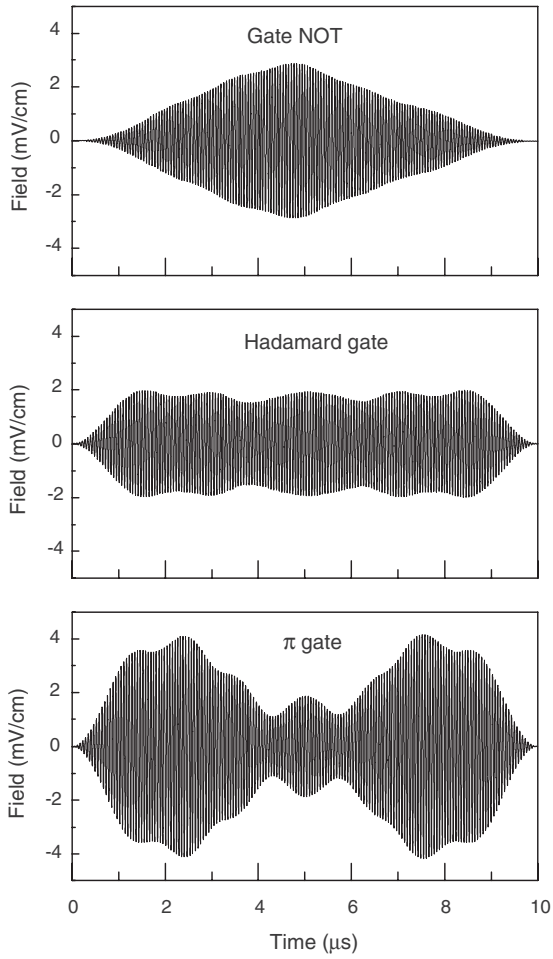

FIG. 5. A set of universal one-qubit gates for $\Delta_z/2\pi=15.5$ kHz. The target time is $T=10$ μs.

the gates NOT, Hadamard transform, and π rotation using the phase-sensitive method [14,16] for unitary transformations. The fidelity $\frac{1}{2}|\Sigma\langle\psi_i(T)|\varphi_f\rangle|^2$ of all three gates was still high, on the order of 0.99, but the pulse shapes for this value of Δ_z were more complicated (see Fig. 5). This demonstrates that if the value of the anharmonicity parameter is chosen too close to the edge of the high fidelity plateau, a significant pulse shaping is necessary in order to achieve accurate qubit transformations.

We also tried to use a different version of the Hamiltonian (2) where the control term is a quadratic function of the distance: $\hat{H}=\hat{H}_0-\frac{1}{2}E_z'(t)z^2q$, which is the simplest example of a spatially inhomogeneous electric field. We found that such a form of the Hamiltonian does not allow controlling transitions between the adjacent states (like $|0\rangle\leftrightarrow|1\rangle$ or $|1\rangle\leftrightarrow|2\rangle$) due to the symmetry properties of the transition matrix elements.

IV. CONCLUSIONS

In summary, we demonstrated that the microwave electric field can be used to coherently control the motion of ions in the anharmonic trap. Creating small anharmonicity

($\Delta_z \sim 1\%$ of ω_z) should permit one to carry out very accurate state-to-state transformations using short ($T \sim 10$ μs) simple-shaped pulses. Amplitude of the electric ac field required for such pulses is on the order of $E_{\max} \sim 2.5$ mV/cm. In general, the values of Δ_z, T, and $E_{\max}$ are all coupled and the pulse optimization is required in order to achieve high fidelity of the state-to-state transformations. This control scheme can be used for state initialization, for simple "cooling," and even for applying the quantum logics gates. Its practical realization seems to be in the reach of today's technology. Note that the gate pulses optimized using the coherent control theory represent unitary transformations, i.e., they preserve phase information and act on an arbitrary superposition state [14,16], which makes this scheme suitable for quantum computation.

When several ions are trapped, a multiqubit system can be created by encoding different qubits into different motional modes of the Wigner crystal (e.g., symmetric and antisymmetric vibration modes). Again, the electric field can be used to control and couple those modes. Note that the single ion addressing is not required for this control scheme. The Coulomb interactions between different ions introduce additional anharmonicities into the spectra of the motional states, which facilitates the control. Recent work on vibrational qubits [13–17] indicates that the two-qubit gates are possible. Optimization of such control pulses is technically feasible, although the pulse shapes may be somewhat more complicated due to the presence of several modes with different frequencies and the interference between multiple transformation pathways. Thus there are no fundamental difficulties for the extension of this theory onto a multi-ion–multiqubit system and we plan to do this in the near future.

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