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Roos, Ingela; Molmer, K

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Quantum computing with an inhomogeneously broadened ensemble of ions: Suppression of errors from detuning variations by specially adapted pulses and coherent population trapping

Ingela Roos[1] and Klaus Mølmer[2]
[1]*Department of Physics, Lund Institute of Technology, Box 118, S-211 00 Lund, Sweden*
[2]*QUANTOP, Danish National Research Foundation Center for Quantum Optics, Department of Physics and Astronomy, University of Aarhus, DK-8000 Århus C, Denmark*

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The proposal for quantum computing with rare-earth-metal-ion qubits in inorganic crystals makes use of the inhomogeneous broadening of optical transitions in the ions to associate individual qubits with ions responding to radiation in selected frequency channels. We show that a class of Gaussian composite pulses and complex sech pulses provide accurate qubit π rotations, which are at the same time channel selective on a 5 MHz frequency scale and tolerant to ± 0.5 MHz deviations of the transition frequency of ions within a single channel. Rotations in qubit space of arbitrary angles and phases are produced by sequences of π pulses between the excited state of the ions and coherent superpositions of the qubit states.

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I. INTRODUCTION

Rare-earth-metal ions doped into inorganic crystals experience inhomogeneous broadening. If the doping concentration is high, a near field probe is able to address individual ions and to induce resonant excitation hopping among nearby ions which can hereby be used for quantum computing [1]. Along similar lines, the rare-earth-metal-ion-doped inorganic crystal proposal for quantum computing (REQC) was developed [2]. Instead of excitation hopping, it uses a dipole blockade mechanism, similar to the Rydberg blockade mechanism for neutral atoms [3], which conditions gate operations on the interaction between a pair of ions exceeding a certain threshold rather than having a precise value. The REQC proposal identifies qubit registers as entire ensembles of collections of interacting ions, selected by their response to radiation at certain frequencies, and distributed over the spatial extent of the crystal.

There is a trade-off between the number of registers accepted by the spectroscopic selection and the precision we can request for their transition frequencies and coupling strengths, and hence, ultimately, between the scalability of the concept and the fidelity of the gate operations. Gate operations are needed that can be carried out with high fidelity, even if the physical parameters of the system are allowed to vary, and following strong and convincing recommendations by Jones [4], we apply composite rotation techniques from liquid and solid state NMR to the problem. Our method, which also involves quantum optical interference techniques, is described in detail for the REQC scheme, but in the conclusion we shall comment on its possible application to a number of other quantum computing proposals.

II. RARE-EARTH-METAL-ION QUANTUM COMPUTING SCHEME

In the rare-earth-metal-ion scheme for quantum computing, qubits are encoded in two ground hyperfine levels $|0\rangle$and $|1\rangle$ of the dopant ions, which are only negligibly disturbed by the interaction with the crystal host. Excited states of the ions interact more strongly with the crystal, and this gives rise to significant broadening of the optical transition between the qubit states and the excited state. The characteristic feature of the proposal is the identification and initialization of the qubits and qubit registers in the crystal: The ith qubit is chosen as the ensemble of ions within the inhomogeneously broadened line which have their absorption frequency at a chosen frequency ν_i. Ions in a frequency window around the qubit channel are pumped to auxiliary states to prevent them from being excited by the near resonant laser light at the qubit frequencies, see Fig. 1.

The excited state of an ion establishes a surrounding permanent dipole field, which shifts the transition frequencies in neighboring ions and which can hence control their interaction with a laser field. Pairs of interacting qubits (i,j) are hence identified, or rather selected, spectroscopically, by pumping away those ions which do not have their transition frequency shifted out of the frequency window around the channel frequency $\nu_{j(i)}$ by the dipole-field, when neighboring ions in the channel $i(j)$ are excited. Physically, the crystal still contains all the ions, but around frequency channels $\nu_{j(i)}$, the ions, populating the qubit levels, are found in close lying pairs, since all ions with insufficient excited state interaction have been deported to passive spectator levels. The

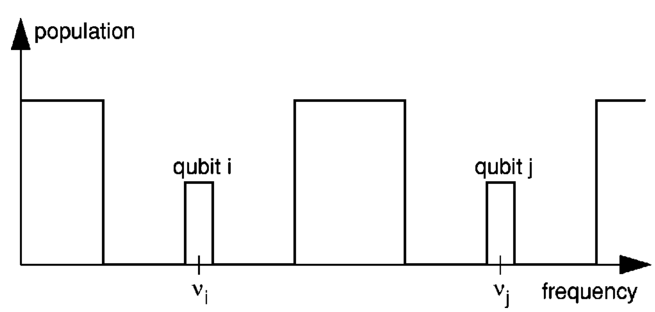


FIG. 1. A schematic diagram of a part of the inhomogeneously broadened spectrum of excitation frequencies to the excited state $|e\rangle$ in rare-earth-metal ions in an inorganic crystal. Two qubits i and j are defined by two different transition frequencies in the spectrally hole-burnt structure.

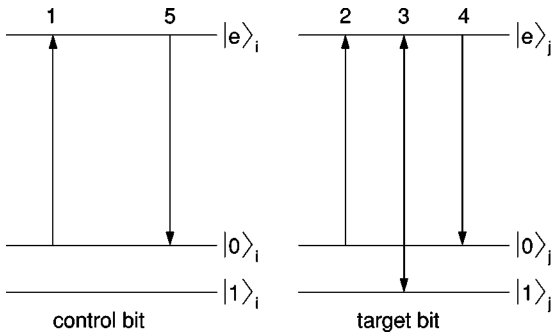


FIG. 2. A CNOT operation with qubit i as control and qubit j as target bit. The operation makes use of the following sequence of π pulses: (1) $|0\rangle_i \leftrightarrow |e\rangle_i$, (2) $|0\rangle_j \leftrightarrow |e\rangle_j$, (3) $|1\rangle_j \leftrightarrow |e\rangle_j$, (4) $|0\rangle_j \leftrightarrow |e\rangle_j$, and (5) $|0\rangle_i \leftrightarrow |e\rangle_i$. See text for explanation.

ensemble of ions in frequency channels ν_i and ν_j thus constitute pairs of mutually interacting ions. Theoretical estimates [2] and preliminary experiments [5] suggest that the dipole energy shifts easily amount to several megahertz, and the ions can be excited with Rabi frequencies in the megahertz range. The homogeneous linewidth is small corresponding to excited state lifetimes on the millisecond scale, whereas the qubit states have lifetimes of seconds with coherence times in the millisecond range with possibilities for increases up to several hundred milliseconds in the presence of magnetic fields [6].

The implementation proposed in Ref. [2] for a controlled-NOT (CNOT) operation, with qubit i as control bit and qubit j as target bit, is shown in Fig. 2. If qubit i is initially in state $|0\rangle_i$, it is excited by the first pulse, and the resulting frequency shift of qubit j makes the steps 2, 3, and 4 nonresonant, hence nothing happens, and qubit i is finally returned to its initial state. If qubit i is in state $|1\rangle_i$, there is no frequency shift, and the resonant processes 2, 3, and 4, effectively exchange states $|0\rangle_j$ and $|1\rangle_j$, as desired for the operation.

III. HIGH-FIDELITY π PULSES

To have a sufficiently large number of active ions, and hence an appreciable number of quantum registers with, e.g., three or more coupled qubits, it is necessary to use ions with frequencies in a not too narrowly defined interval. The widths of the qubit channels, however, imply that the transitions 1–5 in Fig. 2 will not be resonant for all ions, and this seriously compromises the gate fidelity in the system. One could apply very short pulses which are less sensitive to the resonance criterion, but they would excite ions outside the windows around the frequency channels, and they would not display the required sensitivity to the frequency shift on ion j due to the excitation of ion i in the two-bit gate. In a recent paper [7] it was proposed to use a combination of adiabatic processes and coherent control theory to increase the tolerance to variations in physical parameters in a quantum computing model, but very high fidelity was only achieved with very slow processes, which would be compromised by decoherence and decay in the REQC proposal. Instead, we shall present and compare the advantages of two different realizations (composite rotation and complex hyperbolic secant pulse) of π pulses, which rapidly transfer population completely from one state to another in a two-level system, as long as the detuning of the transition lies within a 1-MHz-wide interval, but which does not transfer any population if the detuning exceeds just a few megahertz. Composite pulses were, in fact, already used in quantum computing experiments with trapped ions [8], not to correct for variations in physical parameters, but to obtain π and 4π Bloch sphere rotations on two different transitions where the Rabi frequencies differed by a factor of $\sqrt{2}$. We shall propose a combination of coherent population trapping and π-pulse rotations as a means to make robust qubit rotations through arbitrary angles and on arbitrary qubit states.

A. Composite pulses

Composite pulses can be assigned to two main classes, A and B, where pulses of type A produce a fully compensated rotation of the system for all initial states, whereas pulses of type B provide the compensated transformation only for particular initial states. Levitt [9] has tabulated several sequences of rectangular pulses that provide net 90° and 180° Bloch sphere rotations of two-level systems and which are more tolerant to frequency detunings than a single pulse. Because of the high-frequency components of the rectangular pulses, these pulses do not, however, satisfactorily exclude excitation of the surrounding ions, and we have instead studied composite pulses based on Gaussian field envelopes. On resonance, the accomplishments of a laser pulse is governed only by pulse area and phase, and hence it is natural to replace a rectangular pulse sequence with a sequence of Gaussian pulses with the same areas and phases (θ_k, φ_k), i.e., with the time dependent Rabi frequencies

$$\Omega_R(t) = \sum_k \frac{\theta_k e^{-i\varphi_k}}{\sqrt{2\pi\sigma^2}} e^{-(t-t_k)^2/2\sigma^2}, \quad t \in [t_k - a, t_k + a]. \tag{1}$$

Composite rotations correct errors to high order, and there is a good portion of experience and magic in the design of good sequences. Merely replacing rectangular pulses with Gaussian pulses of equal pulse area and phase therefore does not optimally preserve the error compensating properties. The composite rotation with rectangular pulses, $90_{90}180_0 90_{90}$ [10], provides an error compensated π pulse of type B, and the left panel in Fig. 3 illustrates its tolerance to detuning errors on the 1 MHz scale, but also its erroneous excitation of ions more than 5 MHz away from the channel frequency. Gaussian pulses with the same areas give a better performance without the off-resonant excitations, but we may do even better by slightly adjusting the pulse areas and phases. We have done this in a variational approach, assuming three pulses, and hence six free area and phase parameters. For comparison, we choose the same duration of the rectangular pulse and the Gaussian pulse sequences and a temporal cutoff $a = 3.5\sigma$, so that the pulses are truncated when the amplitude is 0.2% of its maximum. By insisting on perfect operation on resonance and minimum errors for a set of detunings, we have used a variational search to identify an

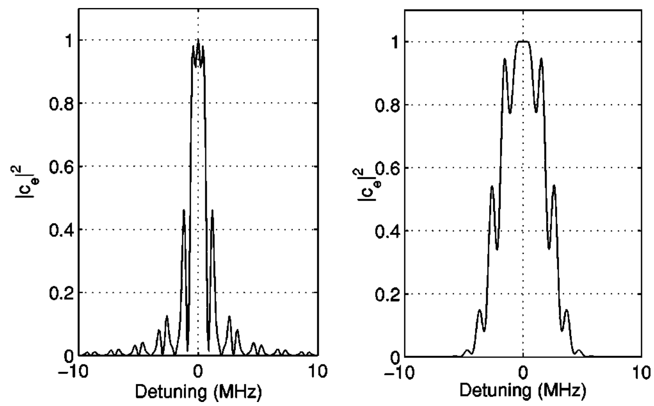


FIG. 3. Excitation by a composite pulse sequence $90_{90}180_{180}90_{90}$ of rectangular pulses (left) and a composite pulse sequence $92.50_{96.98}192.00_{6.86}92.42_{96.23}$ of Gaussian pulses (right). The total duration of both sequences is 1.5 μs.

optimum Gaussian pulse sequence with pulse areas and phases $92.50_{96.98}192.00_{6.86}92.42_{96.23}$. Simulations of the excitation with this composite pulse are plotted in the right panel of Fig. 3. It has been shown [11] that composite pulses can satisfactorily deal with errors in coupling strengths, e.g., due to spatial inhomogeneities of the field strength or variations of the transition dipole moments in the ions, but a gate that works for all input states was not identified in that work, and no solution was presented for the important case of detuning errors in the REQC proposal.

B. Complex hyperbolic secant pulse

As shown by Silver *et al.* [12], complex hyperbolic secant pulses offer an alternative process, of class *B*, with the desired properties. The complex Rabi frequency, $\Omega_R(t)$ of the complex hyperbolic secant pulse is given by

$$\Omega_R(t)=\Omega_0\{\mathrm{sech}[\beta(t-t_0)]\}^{1+i\mu}, \tag{2}$$

where μ is a real constant, Ω_0 is the maximum Rabi frequency, and β is related to the full width at half maxima of the pulse. This corresponds to a real sech pulse envelope in combination with a tanh frequency sweep around the carrier laser frequency ν_L:

$$|\Omega_R(t)|=\Omega_0\mathrm{sech}[\beta(t-t_0)], \tag{3}$$

$$\nu(t)=\nu_L+\mu\beta\tanh[\beta(t-t_0)]. \tag{4}$$

The excitation by such a pulse is shown in Fig. 4 as a function of the detuning $(\nu_L-\nu_i)$. In addition to its favorable tolerance to detuning errors, the complex sech pulse is independent of pulse amplitude if only it exceeds a critical threshold. Its disadvantage compared to the composite Gaussian pulse is the double implementation time.

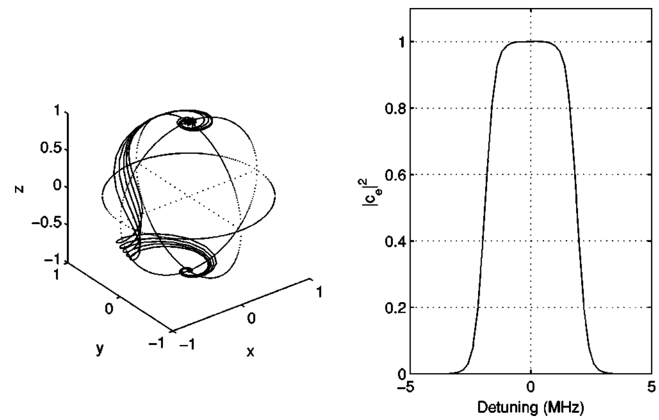


FIG. 4. Excitation by a complex hyperbolic secant pulse for different detunings. The left panel shows the time evolution on the Bloch sphere of ions with different detunings. The right panel shows the excited state population after the pulse as function of detuning. The parameters are $\mu=3$, $\Omega_0=2$ MHz, and $\beta=0.64$ MHz, and the duration of the pulse is 3 μs.

IV. ARBITRARY ROTATIONS, COMPENSATION OF PHASE SHIFTS

A. Using dark states for arbitrary qubit rotations

The pulses described are excellent for steps 1–2 and 4–5 in the CNOT scheme in Fig. 2, since the initial states are explicitly known for all these processes due to the fact that the excited state is unpopulated when the operation starts. The initial state before step 3, however, is an unknown superposition state of $|1\rangle_j$ and $|e\rangle_j$, and a class *A* pulse is required to perform a perfect π pulse on that state. Such composite pulses exist based upon square pulses, but they are difficult to build with Gaussian pulses, and, we also find it difficult to make composite pulses for arbitrary rotations, since the ones provided in the literature often involve a larger number of pulses of which some are rather short, and hence, they will interact with ions outside the hole-burnt structures. Instead, we propose an alternative technique, which does not require class *A* pulses but nevertheless offers robust arbitrary rotations in the qubit space. To this purpose, we shall make use of the full three-level structure of the ions and turn on fields with complex Rabi frequencies $\Omega_{R0}(t)e^{-i\varphi_0}$ and $\Omega_{R1}(t)e^{-i\varphi_1}$ that simultaneously couple $|0\rangle_j$ and $|1\rangle_j$ to $|e\rangle_j$. The system now has two ground-state superpositions, which will be respectively coupled and uncoupled to the excited state. If $\Omega_{R0}(t)=\Omega_{R1}(t)$ we can define a new orthonormal basis according to

$$|\overline{0}\rangle=\frac{1}{\sqrt{2}}\quad(|0\rangle-e^{-i\phi}|1\rangle)$$
$$|\overline{1}\rangle=\frac{1}{\sqrt{2}}\quad(|0\rangle+e^{-i\phi}|1\rangle). \tag{5}$$

If the relative phase of the two fields are chosen so that $\varphi_1-\varphi_0=\phi$, only $|\overline{1}\rangle$ couples to the excited state while $|\overline{0}\rangle$ is a dark state, unchanged by the interaction with the fields, and vice versa if $\varphi_1-\varphi_0=\phi+\pi$. Applying constant phase factors $e^{-i\varphi_0},e^{-i\varphi_1}$ on the sequence of Gaussian pulse or the complex sech pulse described above, we can therefore implement a robust π pulse of class *B*, i.e., from the south pole to the north pole on the Bloch sphere of states $|e\rangle$ and $|\overline{1}\rangle$. If we drive the state back down again by a new π pulse where the constant phase factors of the two fields are both shifted by $\pi+\theta$ in comparison to the first pulse, the net effect becomes a robust phase shift on state $|\overline{1}\rangle$,

$$|\overline{1}\rangle\rightarrow e^{i\theta}|\overline{1}\rangle. \tag{6}$$

In the original qubit basis $(|0\rangle, |1\rangle)$, this procedure is equivalent to the unitary operation

$$U=e^{i\theta/2}\begin{pmatrix} \cos\frac{\theta}{2} & ie^{i\phi}\sin\frac{\theta}{2} \\ ie^{-i\phi}\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}, \tag{7}$$

i.e., a unitary rotation about any axis on the equator of the Bloch sphere representing the qubit state basis. A NOT operation is achieved if θ and ϕ are both set to π, and with three instances of *U*, any unitary rotation in the qubit state basis can be achieved, based exclusively on class *B* π pulses which, in turn, can be implemented in a robust manner by the pulses analyzed in Figs. 3 and 4. A similar combination of coupled and uncoupled superposition states and the stimulated Raman adiabatic passage process was recently proposed [13].

B. Phase compensation

The Bloch sphere rotations introduce detuning and time dependent phases on the individual ions. A phase factor can be considered as global, and thus disregarded only if it appears in front of all qubit states. The two states involved in the above rotations are $|\overline{1}\rangle$ and $|e\rangle$ of the target bit, and one must necessarily arrange for the same phase to be acquired by $|\overline{0}\rangle$. We hence suggest to apply compensating pulses, which have no other effect than to introduce the same detuning dependent phase shift on that state, that is, a composite or complex sech π pulse followed by the inverse π pulse, i.e., with a phase shift of π (but no θ), on $|\overline{0}\rangle\leftrightarrow|e\rangle$. The choice of implementation and the duration of these pulses must be the same as those applied to $|\overline{1}\rangle\leftrightarrow|e\rangle$ for the detuning dependent phases to be accurately compensated.

If the operation is a CNOT operation, i.e., a two-bit operation, we will come across two different detuning dependent phase factors, one dependent on the detuning of the target ion and the other dependent on the detuning of the control ion. Since the detunings, and hence the phase factors, are unknown and not necessarily equal, we have to make sure that every qubit state acquires both phase factors in order to be able to consider the total unknown phase as global. The target qubit rotations, described above, only took place for the state vector components with the control qubit in the state $|1\rangle$, and, thus, conditioned on the control bit being in state $|0\rangle$, we apply a new sequence of compensating pulses to the target states $|\overline{0}\rangle$ and $|\overline{1}\rangle$ so that all states $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$ finally are equipped with the same detuning dependent phases.

TABLE I. Implementation scheme for a robust CNOT operation. Pulses 4 and 5 compensate unknown phase factors, dependent on the detuning of the target bit, caused by pulses 2 and 3. Pulses 7–12 compensate phase factors dependent on the detuning of the control bit, caused by the sequence 1–6. All π pulses should be implemented either as composite pulse sequences or complex sech pulses to yield the desired tolerance to detuning variations.

1	π pulse on $|0\rangle_i\leftrightarrow|e\rangle_i$
2	π pulse on $|\overline{1}\rangle_j\leftrightarrow|e\rangle_j$
3	π pulse on $|\overline{1}\rangle_j\leftrightarrow|e\rangle_j$
4	π pulse on $|\overline{0}\rangle_j\leftrightarrow|e\rangle_j$
5	π pulse on $|\overline{0}\rangle_j\leftrightarrow|e\rangle_j$ (inverse of pulse 4)
6	π pulse on $|0\rangle_i\leftrightarrow|e\rangle_i$ (inverse of pulse 1)
7	π pulse on $|1\rangle_i\leftrightarrow|e\rangle_i$
8	π pulse on $|\overline{1}\rangle_j\leftrightarrow|e\rangle_j$
9	π pulse on $|\overline{1}\rangle_j\leftrightarrow|e\rangle_j$ (inverse of pulse 8)
10	π pulse on $|\overline{0}\rangle_j\leftrightarrow|e\rangle_j$
11	π pulse on $|\overline{0}\rangle_j\leftrightarrow|e\rangle_j$ (inverse of pulse 10)
12	π pulse on $|1\rangle_i\leftrightarrow|e\rangle_i$ (inverse of pulse 7)

V. COMPLETE GATE SEQUENCE, NUMERICAL RESULTS

The implementation scheme for a CNOT operation with qubit *i* as control bit and qubit *j* as target bit is summarized in Table I, and we draw attention to the fact that 12 π pulses (which are all composite or complex sech pulses, but not of class *A*) are applied. This scheme also suffices if the desired gate is a given rotation of the target bit, conditioned on the control bit; only the phase of pulse 3 in the sequence should be adjusted accordingly. Simulations according to this scheme have been performed by solving the equations of motion in the space spanned by the nine states $|a_i b_j\rangle$, where $a,b=0,1,e$. An example of the final state after action of the CNOT operation on an initially entangled state of the qubits is shown in Fig. 5. For simplicity, the detuning parameter was assumed to be the same for the control and target ions in the calculations leading to Fig. 5. The CNOT operation effectively exchanges the amplitudes and hence the populations on states $|10\rangle$ and $|11\rangle$, and this is precisely what we observe for all detunings in the central 1-MHz-wide frequency interval, whereas nothing happens to the state of ions more than 5 MHz away from the exciting lasers. The intermediate frequency intervals are irrelevant, since they contain no ions, see Fig. 1. Decay and decoherence become important on the millisecond time scale, and it is hence important that the gates are fast on this time scale. The total duration of the operation is 18 μs if all π pulses are implemented with composite pulses and 36 μs if they are implemented with complex sech pulses.

In Fig. 6, we show the results of our simulations when the

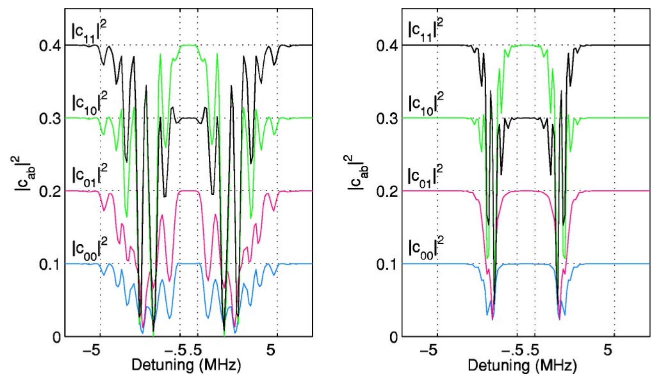


FIG. 5. Simulations of a CNOT operation performed with optimized composite Gaussian pulses (left) and complex sech pulses (right). The initial qubit state was $\psi=\sqrt{0.1}|00\rangle+\sqrt{0.2}|01\rangle+\sqrt{0.3}|10\rangle+\sqrt{0.4}|11\rangle$. The dotted vertical lines represent the edges of the qubit channels and of the spectral hole, respectively. The total duration of the operation is 18 μs if all π pulses are implemented with composite pulses and 36 μs if they are implemented with complex sech pulses.

control and target detunings are allowed to both vary independently within the central 1-MHz-wide frequency channel. The four subplots show the populations, which are also presented in Fig. 5, and we see that the deviations on the edges of the frequency interval are barely 10^{-3} when the 12 π pulses are realized with complex sech pulses whereas implementation with composite Gaussian pulses results in deviations on the order of 10^{-2}. The relative phases between the four states are accurate to the level of 1 deg for both kinds of pulses.

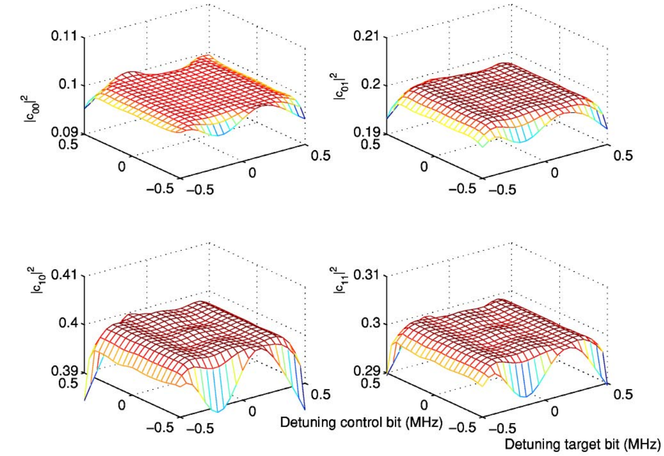
The fidelity of a quantum operation is characterized by the absolute square of the overlap of the quantum state obtained ψ_{out} with the desired quantum state ψ_{ideal}:

$$\mathcal{F}=|\langle\psi_{ideal}|\psi_{out}\rangle|^2=|\langle\psi_{in}|U_{ideal}^{\dagger}U|\psi_{in}\rangle|^2, \tag{8}$$

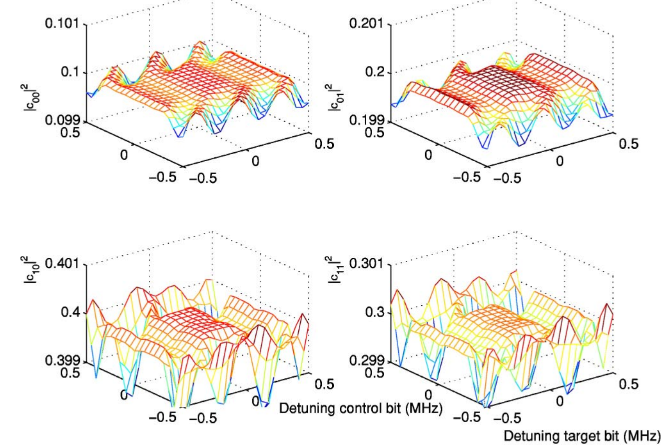
where ψ_{in} is the initial state and the actual and ideal operations are represented by U and U_{ideal}, respectively. The expression $\mathcal{F}$ depends on the input state, and the gate fidelity can be defined as the average or minimum value or some other characteristic estimate of how the gate will perform on an unknown input state. U depends on the detunings of the control and target ions, and we have performed a numerical search for the initial states ψ_{in} minimizing and maximizing the fidelity for different choices of the detuning. Typical values, obtained for detunings -0.3 MHz for the control ion and $+0.5$ MHz for the target ion, are shown in Table II, indicating that the single input wave function applied in Figs. 5 and 6 provides a fair representation of the achievements of our gate.

VI. DISCUSSION

We have shown that composite and complex sech pulses can be applied in combination with coherent population trapping to perform accurate quantum gate operations on ions in the REQC quantum computing proposal. The composite Gaussian pulses do not reach the same high fidelity as the



(a) Composite Guassian pulses



(b) Complex sech pulses

FIG. 6. Simulations of a CNOT operation where the control and target detunings are allowed to vary independently within the qubit frequency channel. The initial state was $\psi=\sqrt{0.1}|00\rangle+\sqrt{0.2}|01\rangle+\sqrt{0.3}|10\rangle+\sqrt{0.4}|11\rangle$ and (a) is realized with composite Gaussian pulses while complex sech pulses are used in (b). Note the different scales.

complex sech pulse. But, they are twice as fast and higher accuracies may be achieved with improved optimization. The combined tolerance to detuning errors on one frequency scale and frequency selectivity on a single order of magni-

TABLE II. Numerically calculated values of the minimum and maximum fidelity of a CNOT operation performed with complex sech pulses and composite Gaussian pulses, respectively. The detuning was set to -0.3 MHz for the control ion and $+0.5$ MHz for the target ion. The fidelity for the initial state $\psi=\sqrt{0.1}|00\rangle+\sqrt{0.2}|01\rangle+\sqrt{0.3}|10\rangle+\sqrt{0.4}|11\rangle$, used in the simulations of Figs. 5 and 6, is also displayed.

	Complex sech pulses	Composite Gaussian pulses
$\mathcal{F}_{min}$	0.997 74	0.971 90
$\mathcal{F}_{max}$	0.999 96	0.999 91
$\mathcal{F}_{\psi}$	0.999 36	0.987 94

tude larger scale are necessary to make quantum computing feasible at all in the REQC proposal, and the first experiments to test our gates are in preparation. Our theory also provide important ingredients for the further development of the proposal, in particular, it contributes significantly to the scalability to larger numbers of coupled qubits.

The achievements of the fault tolerant pulses are remarkable, and it is clear that many quantum optics and quantum information tasks may benefit from their introduction. Other proposals exist for quantum computing where individual addressing of qubits is made spectroscopically, e.g., of optically trapped neutral atoms in inhomogeneous magnetic fields [14], of trapped ions in inhomogeneous magnetic [15], and optical dipole fields [16]. Here, tolerance to variations in the detuning may be desirable as in the present work. Likewise, systems which use spatial addressing may suffer from difficulties of focusing the fields on single qubits, and here tolerance of the relevant qubit to variations around the maximum field and of the neighboring qubits to small variations around the desired vanishing field can be accommodated by only slight modifications of the techniques presented in this paper.

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