Quantum computing in optical microtraps based on the motional states of neutral atoms

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We investigate quantum computation with neutral atoms in optical microtraps where the qubit is implemented in the motional states of the atoms, i.e., in the two lowest vibrational states of each trap. The quantum gate operation is performed by adiabatically approaching two traps and allowing tunneling and cold collisions to take place. We demonstrate the capability of this scheme to realize a square-root of swap gate, and address the problem of double occupation and excitation to other unwanted states. We expand the two-particle wavefunction in an orthonormal basis and analyze quantum correlations throughout the whole gate process. Fidelity of the gate operation is evaluated as a function of the degree of adiabaticity in moving the traps. Simulations are based on rubidium atoms in state-of-the-art optical microtraps with quantum gate realizations in the few tens of milliseconds duration range.

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I. INTRODUCTION

The development of tools to prepare, manipulate and measure the quantum state of a physical system represents one of the great challenges of modern science and, in particular, it is essential for applications in quantum information processing such as quantum computing. At present a few systems have been identified that should permit quantum computation: molecules in the context of NMR\textsuperscript{1}, ion-traps\textsuperscript{2}, cavity QED with photons and atoms\textsuperscript{3}, solid state devices such as quantum dots\textsuperscript{4,5,6}, and trapped neutral atoms\textsuperscript{7,8,9,10,11}. For Rydberg atoms in high Q cavities the engineering of entangled states and the implementation of quantum logic have been demonstrated\textsuperscript{12}; furthermore a quantum gate has been performed between the internal and external degrees of freedom of an ion in a trap\textsuperscript{13}. In NMR systems, quantum algorithms on a few qubits, e.g., Shor’s factoring algorithm, have been reported\textsuperscript{14}.

Neutral atoms are promising candidates for quantum computing for at least two reasons: (i) techniques of cooling and trapping atoms are by now very well established\textsuperscript{15}; and (ii) they are comparatively less sensitive to decoherence, e.g., interaction with the ‘classical’ environment. Neutral atoms can be stored and manipulated in optical lattices\textsuperscript{16}, standard dipole traps\textsuperscript{17}, and microtraps\textsuperscript{18,19,20,21}. In particular, magnetic\textsuperscript{15} and optical microtraps\textsuperscript{19,20,21} offer an interesting perspective for storing and manipulating arrays of atoms with the eventual possibility to scale, parallelize, and miniaturize the atom optics devices needed in quantum information processing. Moreover, optical microtraps can take advantage of the fact that most of the current techniques used in atom optics and laser cooling are based on the optical manipulation of atoms\textsuperscript{17}. Many of the requirements for the implementation of quantum computation\textsuperscript{22} have been recently demonstrated in optical microtraps containing $\sim$ 100 atoms per site\textsuperscript{21}, e.g., selective addressing of single trap sites, and initializing and reading-out of quantum states in each site. In addition, the possibility to store and detect single atoms in optical dipole traps has been reported\textsuperscript{17}.

With the demonstration of single-qubit gates being straightforward, what remains to be experimentally demonstrated is the capability of these optical microtraps to perform two-qubit quantum gates. The most prominent examples of such gates include the CNOT gate, the phase gate and the $\sqrt{\text{SWAP}}$ gate\textsuperscript{4,23}. The latter transforms states $|0\rangle|1\rangle$ and $|1\rangle|0\rangle$, written in the computational basis, to maximally entangled states, while leaving $|0\rangle|0\rangle$ and $|1\rangle|1\rangle$ unaffected, in such a way that after the successive application of two $\sqrt{\text{SWAP}}$ gates the states of the qubits are interchanged. Each one of these two-qubit gates, together with arbitrary single qubit operations, is universal, i.e., allows to perform any quantum algorithm. In practice, the particular two-qubit gate to be implemented will depend on the physical system under consideration.

With respect to neutral atoms, several different physical mechanisms to perform two-qubit gates have been proposed, ranging from cold controlled collisions\textsuperscript{7,8} and dipole-dipole interactions\textsuperscript{3,10,11} to purely geometric quantum evolution\textsuperscript{23}. In the cold collisional case, a two-qubit phase gate was proposed by adiabatically approaching two traps\textsuperscript{7} or by instantaneous state-selective switching of the trapping potentials\textsuperscript{8}. In both cases the qubit was encoded in some internal degrees of freedom of the atoms, e.g., spin, Zeeman or hyperfine levels. For cold collisions to take place the atoms have to be brought to close distances, such that their quantum statistical nature has to be taken into account. A detailed study of the role of the bosonic or fermionic character of
particles in the context of quantum information in atomic waveguide structures has been done by E. Andersson et al. [23, 24].

Here we address the problem of implementing a quantum gate by adiabatically approaching two bosonic atoms, each stored in a different microtrap. In contrast to the proposals mentioned above, we assume the qubit to be implemented in the motional states of the atoms, i.e., an atom in the ground or the first vibrational state of the trap represents $|0\rangle$ or $|1\rangle$, respectively. Note that, as for the ion-trap case, the observation of neutral atoms cooled down to the ground and first vibrational states as well as superposition states in one-dimensional traps has been achieved [27]. To perform the gate operation, we apply the steps outlined in Fig. 1. Initially, the two microtraps are far apart such that the interaction between the two atoms is negligible. Then we adiabatically move both traps close together such that tunneling and cold controlled collisions become important. The dynamics of this process strongly depend on the particular motional state of the atoms and we can make use of this fact to control the interaction such that, after the eventual separation of the traps, the desired gate operation is realized with each trap again containing only one atom.

To be more specific we consider here laser-cooled rubidium atoms stored in optical microtraps [27], assuming that each trap contains initially only one atom. We will show that the $\sqrt{\text{SWAP}}$ gate is the most natural quantum gate to be implemented when the qubit is encoded in the motional states of the atoms and interaction takes place through tunneling and cold collisions. This result applies to both, $^{85}\text{Rb}$ and $^{87}\text{Rb}$, although they have negative and positive scattering length, respectively. In particular, we will demonstrate that a quantum gate of $\sim 20$ milliseconds duration can be performed in state-of-the-art optical microtraps. Very recently, E. Charron et al. [28] have proposed the implementation of a phase gate in an optical lattice with, as it is done also here, the qubit encoded in the motional states. In this case, a controlled interference set-up was proposed to perform a high-fidelity gate with operation time of 38 ms.

The paper is organized as follows. In Section II, we introduce the physical model. Section III is devoted to the implementation of the $\sqrt{\text{SWAP}}$ gate. In Section IV we discuss some practical considerations. And, finally, section V summarizes the results and presents the conclusions.

II. MODEL

In this section we will first write down the Hamiltonian for the two atoms stored in the microtraps and discuss the interaction mechanism. We will introduce a time-dependent orthonormal set of single-particle states for each trap that is also orthogonal to the states of the other trap for arbitrary distances between the two traps. These single-particle states will make it possible to expand the wavefunction in a set of two-particle orthonormal states.

This representation has two important advantages: (i) it allows to compute entanglement throughout the whole gate process; and (ii) it strongly reduces the computational time required to simulate a quantum gate operation with respect to a direct numerical integration of the Schrödinger equation for the two-particle spatial wavefunction. Finally, we will discuss the physical implementation of the qubits and its implications for the quantum gate operations.

A. Hamiltonian

The Hamiltonian governing the dynamics of the two atoms in a time-varying particle-independent trapping potential $V(\vec{r}, t)$ can be written as

$$H = \sum_{i=1,2} \left[ \frac{\vec{p}_i^2}{2m} + V(\vec{r}_i, t) \right] + U(\vec{r}_1 - \vec{r}_2),$$

where $m$ is the mass of the atoms, $\vec{r}_1$ and $\vec{p}_1$ are the (three-dimensional) position and momentum operators for atoms 1 and 2, and $U(\vec{r}_1 - \vec{r}_2)$ accounts for the interaction between the two atoms.

To simplify the problem, we take the trapping potential shape to be time-independent along $y$ and $z$ directions:

$$V(\vec{r}, t) = v(x, t) + v_p(y) + v_p(z),$$

and assume much stronger confinement in $y$ and $z$ directions than in $x$, such that transverse excitations can be neglected. In fact, we will consider that both atoms are cooled down to the $y$ and $z$ vibrational ground states and remain there during all the interaction process. Explicitly, we take the following one-dimensional potential to describe the two microtraps separated by a distance $2a(t)$:

$$v(x, t) = \frac{m\omega^2}{2} \left[ (x + a(t))^2 \theta(-x) + (x - a(t))^2 \theta(x) \right]$$

where $\omega$ is the trapping frequency in the $x$ direction, and $\theta(x)$ is the step function.

The temporary variation of the trap distance is sketched in Fig. 1. Initially the traps are separated by a distance $2a_{\text{max}}$. The process of slowly approaching them to a minimum separation $2a_{\text{min}}$ takes a time $t_r$ and is modeled by the first quarter of a period of a cosine. Then we let the atoms interact for a time $t_i$ and, finally, we slowly separate the traps.

For cold bosonic atoms, the dominant collisional interaction is due to $s$-wave scattering [31], which can be described by a contact potential of the form

$$U(\vec{r}_1 - \vec{r}_2) = \frac{4\pi a_s \hbar^2}{m} \delta^3(\vec{r}_1 - \vec{r}_2),$$
where \( a_t \) is the s-wave scattering length of the rubidium atoms, e.g., in the spin triplet \( a_t = -369 \ a_0 \) for \(^{85}\text{Rb}\) and \( a_t = 106 \ a_0 \) for \(^{87}\text{Rb}\) with \( a_0 \) being the Bohr radius. As long as both atoms remain in the transverse vibrational ground states, we can integrate out the corresponding degrees of freedom and obtain an effective one-dimensional interaction potential \[ u(x_1 - x_2) = 2a_t / h \omega_p \delta(x_1 - x_2), \] where \( \omega_p \) is the transverse trapping frequency. Eqs. (4) and (5) allow us to reduce the complexity of the problem to one dimension.

### B. Single-particle states

We will implement the qubits into the ground and first excited vibrational states of each trap, i.e., we will use the motional states of the atoms. When the two traps are far apart, i.e., \( \alpha a > 1 \) with \( 1/\alpha \equiv \sqrt{\hbar / m \omega_p} \) being the position uncertainty of the ground state, these states are the energy eigenstates of two displaced one-dimensional harmonic oscillators:

\[
\langle x|0\rangle_{L,R} = \frac{\sqrt{\alpha}}{\pi^{1/4}} e^{-\frac{1}{2} \alpha^2 (x \pm a)^2}, \tag{6a}
\]

\[
\langle x|1\rangle_{L,R} = \frac{\sqrt{2\alpha}}{\pi^{1/4}} e^{-\frac{1}{2} \alpha^2 (x \pm a)^2} a(x \pm a), \tag{6b}
\]

with \( L \) and \( R \) labeling the left and right trap, respectively. As we approach the two traps, these single-particle states overlap and are no longer orthogonal. To numerically integrate the Schrödinger equation and to compute entanglement through the gate process, we construct an orthonormal single-particle basis for arbitrary distances of the two traps by applying the Gram-Schmidt method (see Appendix A). If we denote these new single-particle states by \( |\tilde{\ell}\rangle \) with \( \ell = 0, 1, 2, 3... \) and \( s = L, R \) then it holds \( s(|\tilde{\ell}\rangle)_t = \delta_{\ell t} \delta_{st} \). The four states that for large distances correspond to the two lowest states of each trap read

\[
\langle x|0\rangle_{L,R} = \langle x|0\rangle_{L,R} \left[ \frac{\xi^+_{\tilde{\ell}} + \xi^-_{\tilde{\ell}}}{2} \right] + \langle x|0\rangle_{R,L} \left[ \frac{\xi^+_{\tilde{\ell}} - \xi^-_{\tilde{\ell}}}{2} \right] \tag{7a}
\]

\[
\langle x|1\rangle_{L,R} = \langle x|1\rangle_{L,R} \left[ \frac{-x e^{-a^2 \alpha^2}}{\pi^{1/4} \alpha^{3/2}} \langle x|0\rangle_{L,R} \frac{\xi^+_{\tilde{\ell}} + \xi^-_{\tilde{\ell}}}{2} \right]
\]

\[
+ \langle x|1\rangle_{R,L} \left[ \frac{-x e^{-a^2 \alpha^2}}{\pi^{1/4} \alpha^{3/2}} \langle x|0\rangle_{L,R} \frac{\xi^+_{\tilde{\ell}} - \xi^-_{\tilde{\ell}}}{2} \right] \tag{7b}
\]

where \( \xi^+_{\tilde{\ell}}(a) \) and \( \xi^-_{\tilde{\ell}}(a) \) are given in Eqs. (A5). For large separation of the traps, i.e., \( \alpha a \gg 1 \), we have \( \xi^+_{\tilde{\ell}} = \xi^-_{\tilde{\ell}} \) for all \( \tilde{\ell} \) and thus the \( |\tilde{\ell}\rangle_{L,R} \) become the eigenstates of a single harmonic trap centered at \( \mp a \). Notice that the \( |\tilde{\ell}\rangle_{L,R} \) states have the following symmetry under parity transformation: \( \langle x|\tilde{\ell}\rangle_{L,R} \rightarrow (-1)^s \langle x|\tilde{\ell}\rangle_{R,L} \). The general proof is given in Appendix A. This property obviously holds for the \( |i\rangle_{L,R} \) and the \( |\tilde{\ell}\rangle_{L,R} \) are constructed such that this symmetry is maintained.

Although above we have written only four states, for all simulations using these orthogonalized states we will include all states up to \( |\tilde{3}\rangle_{L,R} \).

### C. Two-particle states

Let us motivate the two-particle basis which we will use. On the one hand, it must satisfy bosonic statistics, i.e., the basis states have to be symmetric under the permutation of the particles. On the other hand the Hamiltonian of this system is symmetric with respect to parity transformation, i.e., \( H(x) = H(-x) \), and therefore does not couple states of opposite parity. For this reason we will introduce basis states with well-defined parity. If for this description we limit ourselves again to the four lowest single-particle states, then the bosonic two-particle sector forms a ten-dimensional Hilbert space. Here, we use the following notation \( |\tilde{m}(1)\rangle_s \otimes |\tilde{m}(2)\rangle_t \equiv |\tilde{m}st\rangle \) with 1 and 2 labeling the atoms and \( s, t = L, R \). Thus, the bosonic two-particle basis reads:

\[
|00\rangle^+ = \frac{1}{\sqrt{2}} \left( |0\rangle_L |0\rangle_R + |0\rangle_R |0\rangle_L \right), \tag{8a}
\]

\[
|01\rangle^+ = \frac{1}{2} \left( |0\rangle_L |1\rangle_R + |1\rangle_L |0\rangle_R \right), \tag{8b}
\]

\[
|11\rangle^+ = \frac{1}{\sqrt{2}} \left( |1\rangle_L |1\rangle_R + |1\rangle_R |1\rangle_L \right), \tag{8c}
\]

\[
|\tilde{00}\rangle^+ = \frac{1}{\sqrt{2}} \left( |0\rangle_L |0\rangle_L + |0\rangle_R |0\rangle_R \right), \tag{8d}
\]

\[
|\tilde{01}\rangle^+ = \frac{1}{2} \left( |0\rangle_L |0\rangle_L + |0\rangle_L |0\rangle_L \right), \tag{8e}
\]

\[
|\tilde{11}\rangle^+ = \frac{1}{\sqrt{2}} \left( |0\rangle_R |0\rangle_R + |0\rangle_R |0\rangle_R \right). \tag{8f}
\]
and
\[
|01\rangle^- = \frac{1}{2} \left( |0\rangle_L |1\rangle_R + |1\rangle_L |0\rangle_R \right),
\]
\[
|00\rangle^- = \frac{1}{\sqrt{2}} \left( |0\rangle_L |0\rangle_R - |0\rangle_R |0\rangle_L \right),
\]
\[
|01\rangle^- = \frac{1}{2} \left( |0\rangle_L |1\rangle_R + |1\rangle_L |0\rangle_R \right),
\]
\[
|11\rangle^- = \frac{1}{\sqrt{2}} \left( |1\rangle_L |1\rangle_R - |1\rangle_R |1\rangle_L \right).
\]

The notation at the l.h.s. of Eqs. (8) and (9) means the following: superscripts + or − indicate that the two-particle state has positive or negative parity, respectively, while the tilde accounts for states where, for αa ≫ 1, both atoms are in the same trap, i.e., double-occupancy states. It is easy to check the symmetry of these two-particle states under the exchange of the atoms by making use of the parity property of states |i⟩L,R discussed after Eqs. (7).

In addition it is worth to mention that in our simulations we will consider up to eight single-particle states which give rise to a bosonic two-particle Hilbert space of 36 states (20 states having positive parity from which 10 correspond to double occupancy; and 16 states having negative parity with 10 accounting for double occupancy). Finally note that the fact that we are able to expand the wave-function into this finite number of two-particle orthogonal states has also an important advantage with respect to the time needed for the simulation of a gate operation. We have checked the accuracy of the restriction of the simulation to this subspace by comparing the results of the simulations to a direct numerical integration of the Schrödinger equation for the two-particle spatial wavefunction which is about four orders of magnitude slower.

D. Physical implementation

We start from two well separated traps, each containing one atom. In this situation we can neglect the bosonic nature of the particles and forget about the symmetrization [29]. Only then it is possible to speak about well-defined qubits and we choose to introduce labels A and B for the two qubits by labeling the atom found in the left trap by A and the atom in the right trap by B.

With the two traps far apart, single qubit operations, e.g., a Hadamard gate, can be realized by using two laser pulses in a Raman configuration focused solely on one of the traps. The quantum gate operation between two qubits is much more involved. As we approach the traps, due to tunneling there will be a non-vanishing probability to find both atoms in the same trap. Thus we can no longer distinguish the atoms such that bosonic statistics become important and the qubits are no longer well defined. If, however, we approach and separate the traps in such a way that finally there is again one atom in each of the well separated traps then we can attribute (new) labels A and B to them in the same way as before.

These considerations suggest the following mapping of the states of the computational basis into the two-particle basis states of Eqs. (8) and (9):

\[
\begin{align*}
|0\rangle_A |0\rangle_B & \rightarrow |00\rangle^+ \quad (10a) \\
|0\rangle_A |1\rangle_B & \rightarrow |01\rangle = \frac{1}{\sqrt{2}} (|01\rangle^+ + |01\rangle^-) \quad (10b) \\
|1\rangle_A |0\rangle_B & \rightarrow |10\rangle = \frac{1}{\sqrt{2}} (|01\rangle^+ - |01\rangle^-) \quad (10c) \\
|1\rangle_A |1\rangle_B & \rightarrow |11\rangle^+ \quad (10d)
\end{align*}
\]

Note that the two particle states at the r.h.s of (10) have a trivial evolution at the trapping frequency (or multiples of it) that can be removed by including this phase in the definition of the single particle states.

We will take states (10) as the starting set for the gate operation and, after setting the initial state, we will adiabatically realize the gate. In this adiabatic regime, if we start in an energy eigenstate the system will follow this time-dependent energy eigenstate during the whole gate process. The only allowed transitions are those corresponding to states that (i) are initially degenerate in energy, and, at short distances, (ii) become coupled via tunneling and/or cold collisions. Therefore, in order to find the most suitable gate to be implemented in this system, we have to identify these resonant couplings.

For this aim we will first discuss the ideal case for which there is no interaction between the atoms, i.e. the case where αa = 0 in (8). We then have the following resonant couplings:

\[
\begin{align*}
|00\rangle^+ & \leftrightarrow |00\rangle^+ \quad (11a) \\
|01\rangle & \leftrightarrow |01\rangle \leftrightarrow |10\rangle \leftrightarrow |01\rangle \quad (11b) \\
|11\rangle^+ & \leftrightarrow |11\rangle^+ \quad (11c)
\end{align*}
\]

where |01⟩ = 1 √2 (|01⟩+ + |01⟩−) and |10⟩ = 1 √2 (|01⟩+ − |01⟩−). Therefore, there is a non-negligible probability (even if we move the two traps adiabatically) to have both atoms in the same trap after the gate operation. Note that the kinetic and trapping terms of the Hamiltonian do not directly couple |01⟩ with |10⟩ since they are single particle Hamiltonians and, therefore, they do not allow for the simultaneously change of the motional states of both atoms. The coupling between |01⟩ and |10⟩ is mediated through the double occupancy states |01⟩ and |10⟩. Clearly, in the non-interacting case, a quantum gate operation always has to face with double-occupancy which makes the problem hard to handle.

Figures 2(a) and (b) show, for a particular parameter set, the final state of the system after the whole process of approaching and separating the traps as a function of the scattering length. In (a) the initial state is |01⟩ and in
show that, for couplings read important in the final state of the system. Notice that by changing \( \omega \) can be broken, for instance, by taking an anharmonic trapping potential such that the vibrational frequencies are no longer equally spaced. In addition, it is possible to adjust the interaction time in such a way that, at the end of the gate operation, state \([02]^+\) is not populated. In what follows, we will focus on this last possibility.

III. \( \sqrt{\text{SWAP}} \) GATE

The \( \sqrt{\text{SWAP}} \) gate has the following effect on the states of the computational basis:

\[
\begin{align*}
|0\rangle_A |0\rangle_B & \rightarrow |0\rangle_A |0\rangle_B \\
|0\rangle_A |1\rangle_B & \rightarrow \frac{1 + i}{2} |0\rangle_A |1\rangle_B + \frac{1 - i}{2} |1\rangle_A |0\rangle_B \\
|1\rangle_A |0\rangle_B & \rightarrow \frac{1 - i}{2} |0\rangle_A |1\rangle_B + \frac{1 + i}{2} |1\rangle_A |0\rangle_B \\
|1\rangle_A |1\rangle_B & \rightarrow |1\rangle_A |1\rangle_B
\end{align*}
\]

It is straightforward to check that the successive application of two \( \sqrt{\text{SWAP}} \) gates exchanges the states of the qubits, i.e., \( U_{\text{SWAP}} = U_{\sqrt{\text{SWAP}}} U_{\sqrt{\text{SWAP}}} \). As it has been mentioned before, the \( \sqrt{\text{SWAP}} \) gate together with single qubit operations suffices to realize any quantum algorithm which is not the case for the SWAP gate itself. A simple way to prove this, consists of showing that the universal CNOT gate can be obtained from \( \sqrt{\text{SWAP}} \) gates and single-qubit operations. In fact, a possible sequence is (see Appendix B):

\[
U_{\text{CNOT}} = H_A \sigma_A^1 \sigma_B U_{\sqrt{\text{SWAP}}} \sigma_A^2 U_{\sqrt{\text{SWAP}}} H_A
\]

where \( H_A \) and \( \sigma_{A,B} \) are single-qubit operations. Additionally, sequences involving single-qubit operation exclusively on one of the qubits, e.g., only on A, can be realized [4].

A. Gate simulation

To simulate the gate operation, we have numerically integrated the time-dependent Schrödinger equation for the Hamiltonian given in (3) and (5) with the two-particle wave-function expanded in the previously introduced two-particle basis. Figures 3(a)-(c) show the result of a \( \sqrt{\text{SWAP}} \) gate operation for a scattering length of \( a_s = 106 \) a_0 corresponding to \(^{87}\text{Rb} \) atoms in the spin
FIG. 3: Simulated $\sqrt{\text{SWAP}}$ gate operation for $^{87}\text{Rb}$ with $a_t = 106 \ a_0$. The rest of parameters as in Fig. 2. The initial state of the system is (a) |00$^+$>, (b) |01>, and (c) |11$^+$>. We note that for (b) the final relative phases of |01⟩ and |10⟩ are as in Eq. (13b).

triplet. The parameter setting is as in Fig. 2 and the initial state is (a) |00$^+$>, (b) |01>, and (c) |11$^+$>. The parameter values are chosen to reproduce the gate operation given in (13) as well as to suppress the |02$^+$> population in the outgoing state of Fig. 3(c). Notice that states representing double occupation are populated at close distances for all three cases. However, these populations vanish after the eventual separation of the traps since the traps are moved adiabatically and single-occupation states are not degenerate with double-occupancy ones.

For $^{87}\text{Rb}$ with negative scattering length it is slightly more involved to find parameters for the gate realization since, due to the attractive character of the interaction, double occupation states can more easily become resonant to single occupation states, e.g., |01$^+$> with |00$^+$>. The parameters must be chosen to avoid this degeneracy between double and single occupation states. Fig. 4 shows the result of a gate simulation for $^{85}\text{Rb}$. Unlike for $^{87}\text{Rb}$, Fig. 4(a) shows that starting from |00$^+$> state |01$^+$> is populated during the gate operation.

On the other hand, it is important to notice that the results obtained for $^{87}\text{Rb}$ (Fig. 3) can be also directly implemented in $^{85}\text{Rb}$ by making use of the strong variation of the scattering length in the vicinity of a magnetic field induced Feschbach resonance.

To check the accuracy of the previous simulations in which the two-particle wavefunction was expanded in a finite set of states, we also have numerically integrated the Schrödinger equation for the two-particle spatial wavefunction by using an operator split method and an FFT routine. Fig. 5 shows the results of this integration for the same parameter values as in Fig. 3. The snapshots give the joint-probability distributions for the two particles for three different initial states: (a) |00$^+$>, (b) |01>, and (c) |11$^+$>. The bosonic nature of the atoms manifests in the symmetry of the joint-probability distribution along the diagonal $x_1 = x_2$. In (a) and (c) the final state coincides with the initial one in accordance with Eqs. (13). In (b) |01⟩ evolves towards the maximally entangled state $| (1 + i)|01⟩ + (1 - i)|10⟩⟩/2$ whose joint-probability distribution corresponds to the donut-like shape of the last frame.

The accuracy of the simulated gate operation $U$ with respect to the perfect gate operation $U_{\sqrt{\text{SWAP}}}$ as given by Eqs. (13) is computed through the averaged fidelity.
FIG. 5: Snapshots of the spatial two-particle wavefunction $|\psi(x_1, x_2)|^2$ for $^{87}$Rb. The parameters are as in Fig. 3. The horizontal and vertical axes of each plot show the coordinate of the first and second particle, respectively. Initially there is one particle in each of the traps. The symmetry along the diagonal $x_1 = x_2$ is due to the bosonic statistics. A particle in the ground state of one of the traps corresponds to a gaussian distribution in the direction of the respective axis while one node corresponds to the first excited state. Thus the initial states are (a) $|00\rangle$, (b) $|01\rangle$, and (c) $|11\rangle$. The time for the snapshots is shown in (d). See [31] for animated illustrations of the gate operation.

FIG. 6: Averaged fidelity of the gate operation in the parameter plane $t_r$ versus $a_{\text{min}}$. The interaction time is (a) $\omega_x t_i = 69$ and (b) $\omega_x t_i = 20$. The rest of the parameters as in Fig. 3.

\[ F = \text{Tr}[U \rho U^\dagger U^\dagger \rho U \sqrt{\text{SWAP}}] \] (15)

where the average is taken over the four orthogonal pure input states $\rho$ from Eqs. (13). Figure 6(a) shows for $^{87}$Rb the averaged fidelity $F$ of the gate in the parameter plane $t_r$ versus $a_{\text{min}}$. The rest of the parameters are as in Fig. 3. Clearly, the fidelity is very sensitive to the minimum distance due to the exponential dependence of tunneling at this distance. Note that the fidelity of the gate operation corresponding to the parameters of Fig. 3 is $F \approx 0.9997$ with a gate duration of $2t_r + t_i \sim 17$ ms for $\omega_x = 1.25 \times 10^4$ s$^{-1}$.

An important issue is how much the gate duration can be decreased while maintaining a high fidelity. In Fig. 6(b) the gate duration is reduced by a factor of two which reduces the fidelity by around one order of magnitude. In fact, as soon as the rising time $t_r$ is decreased, non-adiabatic effects occur which in turn result in the population of several unwanted states, e.g. double-occupation, in the final state of the system. However, it could be possible to use the techniques developed in [32] to optimize the speed of the gate operation, while suppressing excitations to these unwanted states.

B. Quantum correlations

Let us briefly consider entanglement in the context of the $\sqrt{\text{SWAP}}$ gate. As already discussed the initial and, as long as double occupancy is suppressed, also the final state consist of well separated and thus for practical purposes distinguishable particles, such that the usual notions of entanglement apply. Let us consider in particular the separable state $|01\rangle$ that under the $\sqrt{\text{SWAP}}$ operation evolves to the maximally entangled state from Eq. (13b). During the operation bosonic statistics become
important and thus we have to distinguish between statistical correlations arising from symmetrization on one hand and quantum correlations which are useful in the context of quantum information on the other hand. Such a distinction has been discussed in [34, 35] for fermionic two-particle states where the notion of Slater rank was introduced and a fermionic measure of entanglement was derived. In [34, 35] these methods have also been used to study correlations in the context of a quantum gate operation for two electrons in quantum dots. They have been translated to bosons in [36] and moreover a bosonic von Neumann entropy has been defined in [33]. Here we want to study to which extent these techniques can be applied to our particular gate operation.

Let us write a general two-boson state in an $N$-dimensional single particle space as $|v⟩ = \sum_{i,j=1}^{N} v_{ij} b_i^\dagger b_j^\dagger |Ω⟩$ where $b_i^\dagger$ and $b_i$ are bosonic creation and annihilation operators and $|Ω⟩$ is the vacuum state such that $b_i^\dagger |Ω⟩ = |i⟩$. The complex symmetric matrix $v_{ij} = v_{ji}$ is normalized as $\text{tr}(v^\dagger v) = 1/2$. If new bosonic annihilation operators $b_i' = \sum_j U_{ij} b_j$ are introduced by a unitary transformation $U$ of the single particle space, then $v$ transforms as $uvU^T$. Now we find that for every symmetric complex matrix $v$ there exists a unitary $U$ such that $uvU^T$ is diagonal, i.e. $uvU^T = \text{diag}[\lambda_1, \ldots, \lambda_r, 0, \ldots, 0]$ with $\lambda_i > 0$. Here $r$ is called the Slater rank of $|v⟩$ and $|v⟩ = \sum_r \lambda_r b_r b_r^\dagger |Ω⟩$ its Slater decomposition.

In our case the initial state $|01⟩$ has Slater rank two while the final state $U_\sqrt{\text{SWAP}} |01⟩$ has Slater rank four. A bosonic measure of entanglement has been proposed that, as a function of the Slater coefficients $\lambda_i$, reads

$$S_B = - \sum_{i=1}^{r} \lambda_i^2 \log_2(\lambda_i^2).$$  \hspace{1cm} (16)

$S_B$ ranges from $S_B = 0$ for states with Slater rank 1 to $S_B = \log_2(N)$ for states with Slater rank $N$ and all $\lambda_i$ equals. For the case considered here we have $S_B(|01⟩) = 1$ and $S_B(U_\sqrt{\text{SWAP}} |01⟩) = 2$. The function $S_B(t)/2$ is plotted in Fig. 6 for the complete $\sqrt{\text{SWAP}}$ operation (the factor is such that $S_B$ for $N = 4$ ranges between 0 and 1). The figure also shows the product $S \cdot p_{\text{single}}$ where $S$ is the von-Neumann entropy calculated by projecting the state onto the space spanned by the set $\{|00⟩^+, |01⟩^+, |01⟩^-, |11⟩^+\}$ and renormalizing. If now states $|i⟩_L$ are considered as being distinguishable from states $|i⟩_R$ then $S$ can be calculated as for distinguishable particles. $p_{\text{single}}$ is the probability to find the state in the space spanned by the given set.

Fig. 7 shows that in the limit of large spatial separation of the particles neither the Slater rank nor the bosonic von Neumann entropy from [33] coincide with the notion of Schmidt rank and von Neumann entropy for distinguishable particles. There are two reasons for this obvious difference: (i) Slater rank and bosonic von Neumann entropy are invariants under arbitrary transformations of the single particle space, while in our case the partition of the full single-particle space into the space spanned by $|i⟩_L$ on the one hand and $|i⟩_R$ on the other is rather fixed; (ii) they do not take into account that here we want to avoid double-occupation in the final state.

In [36] P. Zanardi follows a different approach to calculate an entropy for indistinguishable particles which consists of mapping the bosonic (or fermionic) state to an occupation number basis and calculating the von Neumann entropy in this basis. If this is applied here then the entropy raises from 0 for $|01⟩$ to 1 for $U_\sqrt{\text{SWAP}} |01⟩$ but in between it has a maximum of $\sim 1.4$. As can be seen from the analysis in [37] this is due to the presence of spatial entanglement during the operation. It is however not clear whether this type of entanglement is useful in this context where the two qubits are explicitly implemented in the vibrational states of each trap. These results thus call for further investigation of the problem of quantum correlations in bosonic states.

\section*{IV. PRACTICAL CONSIDERATIONS}

Scalable systems of optical microtraps based on the dipole force can be realized by focusing a single red-detuned laser beam with a micro lens array [13, 21]. The temporal evolution of the trap separation as shown in Fig. 1 can be realized (i) by using two parallel laser beams focused in such a way that the trapping potentials are longitudinally shifted along the common laser beam direction or (ii) by illuminating the micro lens array with
two laser beams under slightly different angles with the possible inclusion of an additional two-dimensional confining potential perpendicular to the direction of the trap displacement [19]. For the parameters we used in the gate simulations, the minimum distance of $a_{\text{min}} \sim 2$ corresponds to a separation of the traps of 1 $\mu$m which is achievable in the present optical microtraps [21]. With laser powers of 1-10 mW per trap, rubidium atoms can be trapped with typical trapping frequencies along the laser beam direction of $\omega_x \sim 10^2$-10$^3$ s$^{-1}$ while the transverse trapping frequencies can be one or two orders of magnitude larger [19]. Additionally, sideband cooling could be applied to cool the atoms to the ground state of each trap in all dimensions.

In the optical microtrap experiments, the trapping potential is gaussian-shaped with typical depths of 1-10 mK $\times k_B$ [19]. For a single trap it is thus a good approximation to assume a harmonic potential for the lower lying states. For two traps being close together the actual potentials will deviate from the form assumed in [19]. Nevertheless, it is possible to generalize the methods applied here to these particular potentials. To allow for single site addressing, typical initial distances between the traps have to be about 5-20 $\mu$m which for rubidium means $a_{\text{max}} = 10 - 40$ instead of $a_{\text{max}} = 5$ which we used in our previous calculations. In this case, it is straightforward to estimate that the process of adiabatically approaching the traps to the interaction distance and eventually separating them again requires another $\sim 10$ ms. Therefore, the whole gate process could be realized in a few tens of milliseconds which is enough for a proof-of-principle experiment. In fact, the lifetime of the atoms in the traps is about 100 – 1000 ms while spontaneous scattering occurs in $\sim 10$ ms. However for strongly confining potentials only a small fraction of the occurring spontaneous scattering processes leads to a change in the vibrational state [19].

In a recent paper, E. Charron et al. [28] proposed the realization of a phase gate in an optical lattice where the qubits were also implemented in the motional states. Two linear counterpropagating beams from the fundamental and first harmonic of a CO$_2$ laser were used to produce an intensity gradient optical lattice. The barrier between two neighboring traps could be raised or lowered by changing the intensity ratio between the two beams. We notice that the realization of a $\sqrt{\text{SWAP}}$ gate as discussed here should also be possible in this setup although the implementation in optical microtraps presents some advantages such as being not sensitive to the phase fluctuations of the lasers.

V. CONCLUSION

We have investigated quantum computation in optical microtraps with the qubits implemented in the motional states of neutral atoms, and tunneling and cold controlled collisions accounting for the interaction between two different qubits. A time-dependent two-particle orthogonal basis has been introduced to simulate the gate operation and to compute entanglement throughout the whole gate process. The bosonic statistic nature of the particles and its role in entanglement has been discussed in detail. We have demonstrated the capability of optical microtraps to realize a high-fidelity $\sqrt{\text{SWAP}}$ gate operation in the few tens of milliseconds range. Finally, some practical considerations for the physical implementation of this quantum gate have been discussed.

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APPENDIX A: GRAM-SCHMIDT ORTHONORMALIZATION

In this appendix we will show how to construct the time-dependent orthonormal single-particle states, denoted by $|i\rangle_L$ and $|i\rangle_R$, from the harmonic oscillator energy eigenstates $|i\rangle_L$ and $|i\rangle_R$ for the left and the right trap, respectively. We start by defining states involving one state of each trap:

$$|i\rangle^\pm \equiv \frac{1}{\sqrt{2}} \left( |i\rangle_L \pm (-1)^i |i\rangle_R \right) \quad i = 0, 1, 2, 3, \ldots$$

(A1)

where the superscript $+$ ($-$) indicates positive (negative) parity with respect to the middle between the two traps. We then group these states according to their parity in two sets $S^\pm = \{ |0\rangle^\pm, |1\rangle^\pm, \ldots \}$ and focus first on the positive parity set $S^+$. This set contains states that are neither orthogonal nor normalized. To perform the orthonormalization, we use the Gram-Schmidt (GM) method starting with the following normalized function:

$$\phi_0^+(x, a) = \frac{\langle x | 0 \rangle^+}{\int \langle x | 0 \rangle^+ \langle 0 | x \rangle^+ dx},$$

(A2)

Then, we define the first linearly independent function $\phi_1^+$ as:

$$\phi_1^+(x, a) = \frac{\langle x | 1 \rangle^+ + a_1 \phi_0^+(x, a)}{\int \langle x | 1 \rangle^+ + a_1 \phi_0^+(x, a) \langle 1 | x \rangle^+ dx},$$

(A3)
where \( a_{10} = -\int \phi_0^+ (x, a) \langle x | 1 \rangle^+ dx \) which guarantees \( \langle \phi_o^+ | \phi_1^- \rangle = 0 \). We repeat this procedure to obtain the rest of the linearly independent functions \( \phi_2^+, \phi_3^+, \ldots \) with positive parity. In an analogous way, we determine from \( S^- \) the set of linearly independent functions \( \{ \phi_0^-, \phi_1^-, \phi_2^-, \phi_3^-, \ldots \} \). An important feature of the GM method when applied to a set of states with the same parity is that the constructed orthonormal states retain the parity of the original set of states. Thus states from \( \{ \phi_0^+ \} \) and \( \{ \phi_1^+ \} \) have positive and negative parity, respectively, and, therefore, the whole set \( \{ \phi_0^+ , \phi_1^+ , \phi_2^+ , \phi_3^+ , \ldots \} \) is orthonormal. Explicitly, the first four orthonormalized functions read

\[
\begin{align*}
\phi_0^+ (x, a) &= \xi_0^\pm (a) \langle x | 0 \rangle^\pm, \\
\phi_1^+ (x, a) &= \xi_1^\pm (a) \left( \langle x | 1 \rangle^\pm \mp \frac{a^3}{4} e^{-a^2} | 0 \rangle \langle 0 | x \rangle \right)
\end{align*}
\]

where

\[
\begin{align*}
\xi_0^\pm (a) &= \frac{1}{\sqrt{1 \pm e^{-a^2/\alpha^2}}}, \\
\xi_1^\pm (a) &= \frac{e^{a^2/2}}{\sqrt{a^2 (e^{a^2} - e^{-a^2}) + 2a^2}}
\end{align*}
\]

For the sake of brevity, we do not explicitly show the analytical expressions for the rest of the \( \phi_i^\pm \).

Once we have obtained the orthonormal set \( \{ \phi_i^\pm \} \), it is straightforward to write down the single-particle basis that we will use:

\[
\begin{align*}
\langle x | i \rangle_L &= \frac{1}{\sqrt{2}} (\phi_i^+ + \phi_i^-), \\
\langle x | i \rangle_R &= (-1)^i \frac{1}{\sqrt{2}} (\phi_i^+ - \phi_i^-)
\end{align*}
\]

These states are orthonormal due to the orthonormality of the \( \phi_i^\pm \) and in the limit \( a^2 \alpha \gg 1 \) become the corresponding harmonic oscillator energy eigenstates for each trap. These new orthonormal states do not have in general a well defined parity with respect to the center of the corresponding trap but it is straightforward to check from Eqs. (A6) that they satisfy the following property under parity transformation with respect to the middle of the traps:

\[
\langle x | i \rangle_{L,R} \rightarrow (-1)^i \langle x | i \rangle_{R,L}.
\]

**APPENDIX B: UNIVERSALITY OF THE \( \sqrt{\text{SWAP}} \) GATE**

Our goal here is to write down the sequence of steps required to build the CNOT gate, which, in the computational basis \( |0\rangle_A |0\rangle_B, |0\rangle_A |1\rangle_B, |1\rangle_A |0\rangle_B \) and \( |1\rangle_A |1\rangle_B \), reads

\[
U_{\text{CNOT}} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}, \tag{B1}
\]

from the \( \sqrt{\text{SWAP}} \) gate

\[
U_{\sqrt{\text{SWAP}}} = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1+i}{\sqrt{2}} & \frac{1-i}{\sqrt{2}} & 0 \\
0 & \frac{1-i}{\sqrt{2}} & \frac{1+i}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}. \tag{B2}
\]

The single qubit operations we need are on one hand the Hadamard gate

\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
1 & -1
\end{pmatrix}, \tag{B3}
\]

and on the other hand the following combination of identity and Pauli \( \sigma_z \) matrices:

\[
\sigma = \begin{pmatrix}
1 & 0 \\
0 & -i
\end{pmatrix} = e^{-i \frac{\pi}{4} \sigma_z}, \tag{B4}
\]

Let us call \( H_{A,B} \) and \( \sigma_{A,B} \) the corresponding single-qubit operations for qubit A or B. Now it is easy to check that the following combination of single-qubit operations and \( \sqrt{\text{SWAP}} \) gates yields the phase gate:

\[
U_{\text{Phase}} = \sigma_A^{-1} \sigma_B U_{\sqrt{\text{SWAP}}} \sigma_A^2 U_{\sqrt{\text{SWAP}}^2}, \tag{B5}
\]

This sequence is not unique, and more sophisticated sequences involving single-qubit operations on only one of the qubits can be implemented \( \text{[4]} \). Finally, to obtain the CNOT gate it is enough to apply a Hadamard gate on the qubit A at both sides of Eq. (B3), i.e.

\[
U_{\text{CNOT}} = H_A U_{\text{Phase}} H_A. \tag{B6}
\]
