Quantum computing implementations with neutral particles

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We review quantum information processing with cold neutral particles, that is, atoms or polar molecules. First, we analyze the best suited degrees of freedom of these particles for storing quantum information, and then we discuss both single- and two-qubit gate implementations. We focus our discussion mainly on collisional quantum gates, which are best suited for atom-chip-like devices, as well as on gate proposals conceived for optical lattices. Additionally, we analyze schemes both for cold atoms confined in optical cavities and hybrid approaches to entanglement generation, and we show how optimal control theory might be a powerful tool to enhance the speed up of the gate operations as well as to achieve high fidelities required for fault tolerant quantum computation.

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I. INTRODUCTION

Since the 1990s, when groundbreaking algorithms based on the laws of quantum mechanics for solving classically intractable computational problems were found, quantum information science has rapidly grown with the promise to build up a quantum computer. Similar to nowadays “classical” computers, quantum hardware consists of a memory and a processor. The former stores the information, the latter, with a set of gates, processes the information.

The concept of gate is fundamental in quantum computation \cite{1}, and therefore we first consider its classical analogue. A gate on a classical computer, which implements a Boolean function, is a device that accomplishes a well-defined operation on one or more bits. For instance, CMOS transistors realize the logical NOT operation. Instead, a quantum gate performs a unitary transformation on the linear space of quantum bits (qubits). Thus, a quantum gate is the time propagator generated by a given Hamiltonian; control by external fields, according to the Hamiltonian structure, allows to perform desired transformations on the qubit wave function. Again in the 90s it has been showed that a general \( N \)-qubit gate can be decomposed into \( O(N^3) \) one- and two-qubit gates. As a consequence, most of the schemes for quantum gates concern the implementation of one- and two-qubit operations.

Neutral particles such as cold atoms and polar molecules are excellent candidates for quantum information processing (QIP) implementations. Indeed, (i) they have exquisite coherence properties; (ii) their coherent evolution can be accurately controlled in tailored micropotentials; and (iii) they present the exciting perspective of interfacing their qubit degrees of freedom with solid-state systems.

There are two main paradigms for a quantum hardware based on neutral particles in surface traps: the first one is a microfabricated device called atom chip, whereas the second one relies on the combination of both polar molecules and superconducting circuits. In figure the general idea of an atom chip quantum processor is illustrated. It includes a reservoir of cold atoms, preferably in their motional ground state, and in a well-defined internal state. An ideal starting point for this is a Bose-Einstein condensate (BEC) in a chip trap. From there the atoms are transported using guides or moving potentials to a large array of processing sites. Either single atoms, or small ensembles of atoms, are then loaded into the qubit traps. Each qubit site can be addressed individually. Microfabricated wires and electrodes located close to the individual sites can be used for site-selective manipulations such as single-qubit gates. For two-qubit gates, interactions between adjacent sites are induced. For readout, micro-optics can be used to focus lasers onto each site separately, or the whole processor can be illuminated and single qubits are addressed by shifting them in and out of resonance using local electric or magnetic fields.

The other model of quantum computation is illustrated...
II. SUITABLE QUBIT STATES FOR QIP

Two potentially conflicting requirements have to be met by the qubit states \{\ket{0}, \ket{1}\} chosen for QIP with neutral particles. On the one hand, both states have to couple to the electromagnetic fields which are used for trapping and manipulating, for example, the atoms. On the other hand, high-fidelity gate operations require a long coherence lifetime of superposition states \(\alpha\ket{0} + \beta\ket{1}\), \((|\alpha|^2 + |\beta|^2 = 1)\), and thus the qubit has to be sufficiently robust against fluctuations of electromagnetic fields in realistic experimental situations. A peculiarity of chip-based traps is the presence of atom-surface interactions, which lead to additional loss and decoherence mechanisms which are not present in macroscopic traps. It is therefore important to investigate the coherence properties of the proposed qubit candidates close to the chip surface. In the following we discuss the different types of qubits which have been studied.

A. Hyperfine qubits

An obvious qubit candidate are the long-lived (electronic) ground state hyperfine levels of the atoms. In most experiments, at least a part of the trapping potential is provided by static magnetic fields generated by wires or permanent magnet structures on chip. It is therefore desirable that both \(\ket{0}\) and \(\ket{1}\) are magnet-
ically trappable. Long coherence lifetimes can be expected if states with equal magnetic moments are chosen, so that both states experience nearly identical trapping potentials in static magnetic traps, and the energy difference $h
u_{10} = E_{1} - E_{0}$, between $|0\rangle$ and $|1\rangle$ is robust against magnetic field fluctuations. These requirements are satisfied by the $|F = 1, m_F = -1\rangle \equiv |0\rangle$ and $|F = 2, m_F = +1\rangle \equiv |1\rangle$ hyperfine levels of the $5S_{1/2}$ ground state of $^{87}\text{Rb}$.

In Ref. [10], the coherence properties of this qubit pair were studied experimentally on an atom chip. A coherence lifetime exceeding 1 s was measured at different atom-surface distances using Ramsey spectroscopy. These experiments confirm that this hyperfine qubit is very well suited for atom-chip based QIP. It is therefore considered in several schemes for quantum gates and we shall describe gate implementations using this qubit in some detail later in the paper.

Magnetic field insensitive hyperfine qubits were also experimentally studied in optical microtraps, created by an array of micro lenses [11]. Using spin-echo techniques, coherence times of 68 ms were obtained, limited by spontaneous scattering of photons. Simultaneous Ramsey measurements in up to 16 microtraps were performed, demonstrating the scalability of this approach.

Finally, we also note that by using alkaline-earth(-like) atoms one can encode qubits in nuclear spin states, decoupled from the electronic state in both the $1S_0$ ground state and the very long-lived $3P_0$ metastable state [12].

B. Motional qubits

Qubits can also be encoded in the vibrational states of atoms in tight traps. This has been proposed both for optical [13, 14] and magnetic [15, 16] microtraps. The computational basis states can be two vibrational levels in a single trap, e.g. the ground and first excited vibrational level [13]. Alternatively, they can be defined by the presence of an atom in either the left or the right well of a double well potential [13]. Initialisation of the atoms in the lowest vibrational state of the trap with high fidelity is crucial in both of these schemes.

Vibrational states are usually more delicate to handle and to detect than hyperfine states. An advantage, on the other hand, is that an internal-state independent interaction is sufficient for two-qubit gates and collisional loss can be reduced as the two interacting qubits are in the same internal state. The proposals of Refs. [15, 16] therefore consider a combination of hyperfine states for qubit storage and vibrational states for processing. Measurements of vibrational coherence near surfaces still have to be performed. The expected fundamental limits due to surface-induced decoherence, however, are comparable to those for hyperfine states.

C. Rydberg state qubits

Rydberg states are attractive for QIP because of their strong electric dipole moment [17, 18]. The resulting dipole-dipole interaction between Rydberg atoms can be exploited for fast two-qubit quantum gates. Moreover, Rydberg qubits can be combined with long-lived ground state hyperfine qubits for information storage. For the $n \sim 50$ Rydberg states of Rb, typical lifetimes are $\sim 100 \mu s$ for low angular momentum states up to $\sim 30$ ms for circular states. In Ref. [18] it is proposed to enhance the lifetime of circular Rydberg states into the range of seconds by using a microstructured trap on a superconducting (atom) chip that simultaneously acts as a cavity with a microwave cut-off frequency high enough to inhibit spontaneous emission. Furthermore, it is shown that with the help of microwave state dressing, coherence lifetimes of similar magnitude could be achieved.

D. Ensemble-based qubits

A single qubit can be encoded in collective states of an ensemble of particles [19, 20]. State $|0\rangle$ corresponds to all particles in the ground state, while in state $|1\rangle$, a single excitation is shared collectively by the whole ensemble. To isolate this two-level system, a blockade mechanism is required that prevents the creation of two or more excitations. The necessary nonlinearity can be provided by the dipole-dipole interaction of Rydberg atoms [19–21], or by coupling the ensemble via a cavity to a single saturable two-level system such as a Cooper pair box [3, 22]. Ensemble qubits have the advantage that single-atom preparation is not required. Moreover, the Rabi frequency between the collective qubit states is enhanced by $\sqrt{N}$, where $N$ is the number of atoms in the ensemble. The decay rates are the same as for a single particle if the decay is dominated by non-collective processes such as atom loss. Ensemble qubits in chip traps have been considered for ground state atoms [22], Rydberg atoms [21], polar molecules [3, 23], and electron spins [24]. Recently, for the latter, an experiment demonstrates the storage and retrieval of up to 100 weak 10 GHz coherent excitations in such collective qubit states [25].

III. SINGLE-QUBIT OPERATIONS

Single-qubit gates are unitary transformations in the Hilbert space of a single qubit. The necessary degree of control can be experimentally demonstrated by driving high-contrast Rabi oscillations between the qubit states. Atom-chip based experiments have demonstrated such control with hyperfine qubit states. Coherent control of motional states has been demonstrated in the context of atom interferometry. Given that, in this section we only focus on hyperfine and motional qubit states. Beside this, the schemes based, for instance, on Rydberg states,
utilize similar methods and (experimental) techniques for implementing single qubit rotations than those described here.

### A. Hyperfine qubits

Hyperfine qubit states can be coupled with oscillating microwave and/or radio frequency (rf) magnetic fields. High fidelity Rabi oscillations on the qubit transition $|0\rangle \equiv |F = 1, m_F = -1\rangle \leftrightarrow |1\rangle \equiv |F = 2, m_F = +1\rangle$ of $^{87}$Rb, whose first order Zeeman shift is approximately identical, have already been demonstrated experimentally on an atom chip [26]. In this case, a two-photon transition with a microwave and an rf photon is involved. A two-photon Rabi frequency of a few kHz is easily achieved, so that single-qubit gates can be performed on a time scale of hundreds of microseconds (with a $\pi$-pulse fidelity of $> 96\%$), three to four orders of magnitude faster than the relevant coherence lifetimes. Alternatively, hyperfine states can be coupled through a two-photon Raman transition driven by two laser beams [11, 27].

We note that in atom-chip systems the qubit driving fields can be generated by chip-based waveguides (for microwaves) or just simple wires (for rf). This results in a stable, well-controlled coupling with tailored polarization. All elements for qubit manipulation can thus be integrated on chip. Moreover, chip-based driving fields can have strong near-field gradients. This is advantageous as it allows individual addressing of spatially separated qubits. On the other hand, care has to be taken to avoid dephasing due to strong gradients across a single qubit.

The above discussion concerns implementations in atom-chip systems, but, as we shall discuss in Sec. VI, optical lattices offer also an interesting platform for carrying out QIP protocols, especially because with them it is possible, simultaneously, to coherently manipulate millions of qubits [28]. The detection and manipulation of a single atom amongst an ensemble of $\sim 10^5$ atoms presents more difficulties than in an atom chip. Since the addressing occurs with a focused laser beam, the spacing between (nominally) identical lattices sites has to be larger than the optical diffraction limit, or, alternatively, arrays of independent single-atom traps sufficiently spaced can be used [29–31]. The drawback of such approaches, however, is the need to use non-clock states, that is, field-sensitive states, thus with shorter coherence times, a requirement that is conflict with the third Di-Vincenzo criterion for quantum computing [3], namely (i) in our introduction. Recently, however, it has been shown, that in addition to the aforementioned qubit pair states, used to store the information, the field insensitive pair $|0\rangle \equiv |F = 2, m_F = 0\rangle \leftrightarrow |1\rangle \equiv |F = 1, m_F = 0\rangle$ of $^{87}$Rb (referred to as “working” states) enables to obtain a fidelity for single qubit operations also larger than $96\%$ [32]. This can be achieved by mapping a superposition state of a storage qubit to the corresponding working states, because while the transitions $|0\rangle \leftrightarrow |1\rangle$, $|0\rangle \leftrightarrow |1\rangle$ are insensitive to external fields, the transitions $|0\rangle \leftrightarrow |0\rangle$, $|1\rangle \leftrightarrow |1\rangle$ are instead field sensitive. The application of a magnetic field gradient, which shifts the energy levels (Zeeman effect), allows to spectrally select a particular qubit from the quantum register. Field-sensitive transitions can then be used to transfer the storage-state superposition to the pair of working states for the selected qubit register with a fidelity of $99\%$. At this point, an arbitrary qubit rotation can be performed on the selected qubit alone, since the working-state transition is off-resonant from the storage-state transition. Then, the inverted transfer process returns the selected qubit register to a new storage-state superposition. Such a technique is quite interesting and promising, because the spatially inhomogeneous external magnetic field used to map a storage-state superposition of the selected qubits to a working-state superposition, with a minimal perturbation of the unselected qubits, is not spatially localized. Hence, such a procedure makes the addressability of qubits less complicated while decoherence effects are substantially suppressed.

Finally, we underscore that recently also single atom addressability in a two-dimensional geometry has been experimentally achieved, by using either a tightly focused laser beam together with a microwave field [33] or by means of techniques from solid immersion microscopy [34]. These results have demonstrated a subdiffraction-limited resolution, significantly below the lattice spacing.

### B. Motional qubits

If the qubit is encoded in the ground and first excited vibrational levels of a single trap [13, 15, 16], qubit rotations can be induced by driving a two-photon Raman transition between the states with two lasers. Such transitions between vibrational levels are routinely employed in ion trap QIP [27] and have been demonstrated in optical dipole traps [33]. Similar experiments with neutral atoms in chip traps still have to be performed. As the vibrational levels have to be spectrally resolved, tight traps with large vibrational frequencies are required. On atom chips, sufficiently high vibrational frequencies of up to $\sim 1$ MHz are accessible. If the qubit basis states are the left and right states of a double well [14], single-qubit gates can be performed by adiabatically lowering the barrier between the two wells and allowing tunneling to take place. This has strong connections to atom interferometry. Chip-based atom interferometers demonstrating versatile coherent control of the motional state of BECs have been realized, see e.g. [20, 30, 37].
IV. CONDITIONAL DYNAMICS

Two-qubit gates are the heart of a quantum processor, as they are required for the generation of entanglement between the qubits.

Let us consider the dynamics of an arbitrary number of particles (no matter if charged or not) in a time- and state-dependent three-dimensional trapping potential $V_k(r,t)$ $[r=(x,y,z)]$ governed by the Hamiltonian operator $[38, 39]

\[ \hat{H}(t) = \frac{1}{2m} \int dr \hat{\Psi}_k^\dagger(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_k(r,t) \right) \hat{\Psi}_k(r) \]

\[ + \frac{1}{2} \sum_{k,\ell=0}^{1} \int dr dr' \hat{\Psi}_k^\dagger(r) \hat{\Psi}_\ell^\dagger(r') U_{k\ell}(r,r') \hat{\Psi}_\ell(r') \hat{\Psi}_k(r) . \]

(1)

Here $m$ is the mass of the particle, $\hat{\Psi}_k^\dagger(r)$, $\hat{\Psi}_k(r)$ are field creation and annihilation operators for the logic state $|k\rangle$, and $U_{k\ell}(r,r')$ is the two-body interaction potential for the qubit states $|k\rangle$ and $|\ell\rangle$, with $k, \ell = 0, 1$. Our goal is the realization of a two-qubit gate with two neutral particles (e.g., atoms), each of them carrying a qubit of information usually encoded in an extra degree of freedom (e.g., a pair of hyperfine states) other than their motional state. In this specific case, the full many-body problem described by the Hamiltonian [41] can be reduced to a Schrödinger equation for two trapped particles and this will be assumed in the following.

The quantum gate we aim to implement is a phase gate having the following truth table: $|e_1\rangle|e_2\rangle \rightarrow e^{i\phi_2}|e_1\rangle|e_2\rangle$, where $|e_1\rangle, |e_2\rangle$ are the logic qubit states with $e_1, e_2 = 0, 1$. When the phase $\phi_2$ takes on the value of $\pi$, the combination of a phase gate with two Hadamard gates yields a controlled-NOT gate. In this respect it is an important quantum gate. Since it requires only to produce a phase shift for the state $|1\rangle|1\rangle$ such a gate has become of interest, because it requires a state-dependent interaction that is relatively straightforward to realize physically.

Let us explain the basic principle to obtain a conditional phase shift $\phi_g$ when two neutral particles are trapped in a microscopic potential. Initially, at $t = 0$, we assume that the two particles are in the respective ground states of the trapping potential and that their wave functions are well separated from each other so that their overlap is negligible. At times $0 < t < \tau_g$ the potential wells are changed in such a way that the particle wave functions are displaced differently depending on their logical state $|k\rangle$ and a state-dependent wave function overlap results.

The particles interact for a time $\tau_g$, the gate operation time, and at $t = \tau_g$ the initial situation is restored. With this approach we get state dependent phase shifts of two kinds: a purely kinematic one, $\phi_k + \phi_\ell$, due to the single particle motion in the trapping potential; and an interaction phase, $\phi_{k\ell}$, due to the coherent interactions among the particles. Thus, we can summarize the ideal phase gate with the mapping $[39, 40, 41]

\[ |e_1\rangle|e_2\rangle \rightarrow e^{i\phi_{e_1e_2}}|e_1\rangle|e_2\rangle, \]

(2)

where the motional state $|\psi_{e_1e_2}\rangle$ has to factor out at the beginning and at the end of the gate operation. In the ideal transformation (2) we grouped together the kinematic and global two-particle phases. Indeed, the application of single-qubit operations affords $\phi_g = \phi_{11} - \phi_{01} - \phi_{10} + \phi_{00}$ [41].

We conclude this section by introducing the concept of gate fidelity $F \in [0,1]$, which will be a useful quantity later to assess the gate performance. Basically, it is the projection of the physical state obtained by actually manipulating the system onto the logical state that the gate aims to attain, averaged over degrees of freedom (e.g., motion) that cannot be accurately controlled.

V. TWO-QUBIT GATES BASED ON COLLISIONAL INTERACTIONS

In this section we analyze in some detail two important groups of gate schemes with neutral atoms that are well suited for atom chip based implementations: the first one encodes the quantum information in internal levels of the atoms, and utilizes the external (motional) degrees of freedom to manipulate the information; the second one, instead, stores the information in the external degrees of freedom and the internal ones might be used to process it. Importantly, in both scenarios, the entanglement between the qubits is produced by the collisions among the atoms.

In order to obtain conditional dynamics, as we discussed in the previous section, either the trapping potential or the interaction term should be state-dependent. In the case of ultra-cold neutral atoms, the interaction between atoms is mediated by two-body collisions, whose dominant contribution is s-wave scattering described by

\[ U_{k\ell}(r,r') = \frac{4\pi\hbar^2a_s^{k\ell}}{m}\delta^3(r-r'), \]

(3)

where $a_s^{k\ell}$ is the s-wave scattering length for the internal states $|k\rangle$ and $|\ell\rangle$. Due to the short range of the pseudopotential (3), the wave functions of the atoms have to overlap in order to interact, and for identical atoms in the same logical state, s-wave scattering is only possible for bosons, and therefore in the following we will consider bosonic atomic species. As the potential given in Eq. (3) assumes elastic collisions, the states $|0\rangle$ and $|1\rangle$ have to be chosen such that they remain the same after the collision.
A. Internal-state qubits

One of the most effective theoretical models for an atom chip phase gate has been proposed in Ref. [38]. In this scheme the control of the interaction between the atoms is realized by changing the shape of a microscopic potential depending on the internal state of the atoms. Three conditions are assumed: (i) the shape of the potential is harmonic; (ii) the atoms are initially cooled to the vibrational ground state of two potential wells centered at \( r = r_0 \) and \( r = -r_0 \); (iii) the change in the form of the trapping potential is instantaneous. The principle of the gate is the following: at time \( t = 0 \) the barrier between the atoms, say in the \( x \) direction, is suddenly removed (selectively) for atoms in the logical state \( |1 \rangle \), whereas for atoms in the internal state \( |0 \rangle \) the potential is not changed. An atom in the logical state \( |1 \rangle \) finds itself in a new harmonic potential centred at \( r = 0 \) with a frequency \( \omega \), smaller than the one of the separated wells, \( \omega_0 \). The atoms in state \( |1 \rangle \) are allowed to perform an integer number of oscillations and at \( t = \tau_g \) the initial wells are restored. In this process the particles acquire both a kinematic phase due to their oscillations in the traps and an interaction phase due to their collisions. In the tight transverse confinement regime, where the frequency \( (\omega_\perp) \) of the well in the \( y, z \) directions is much larger than that \( (\omega, \omega_0) \) in the \( x \) direction, the gate dynamics can be well approximated by a one-dimensional (1D) model with a contact potential \( U_{kl}^{1D}(x, x') = 2\hbar \omega_j a_{kl}^j s(x - x') \) [12]. The kinematic phase \( 2\pi \omega_\perp / \omega (\tau_g = 2\pi n / \omega, n \in \mathbb{N}) \) due to the radial confinement is common to all states, while the one due to the oscillation in the axial direction is state dependent. Due to the harmony of the trapping potentials, almost perfect revivals of the wave packet occur. By choosing \( \omega = \omega_0 / j \), with \( j \in \mathbb{N} \), and in the limit where the interaction does not induce any relevant alteration in the shape of the two-particle wave function, the gate operation time \( \tau_g \) can be fixed by looking at the revival where the total accumulated phase \( \phi_g \) assumes a defined value, e.g., \( \pi \). Due to the form of \( U_{kl}^{1D} \), the frequency \( \omega_\perp \) can be adjusted in order to fix the value of \( \phi_g \) [38].

Atom chips can provide microscopic state dependent potential landscapes in which atoms can be trapped and manipulated for the implementation of the above scheme. In Ref. [2] it was pointed out that a combination of static magnetic and static electric fields could be used for this purpose. However, several issues have to be addressed that could prevent a successful experimental realization of the scheme discussed above: (i) the trapping potentials are usually anharmonic; (ii) the fidelity is strongly reduced by wave packet distortion due to undesired collisions in some of the qubit basis states [38]; (iii) transverse excitations of the atoms can arise during the collisions if the ratio \( \omega_\perp / \omega \) is not properly chosen for the 1D condition. Those processes would significantly reduce the gate fidelity.

An analysis of the limitations due to anharmonicity of the potentials is carried out in Ref. [43]. In that analysis a cubic and a quartic term is added to the harmonic potential in order to include the next leading order terms in the Taylor series expansion of an arbitrary potential. While a cubic anharmonicity is well tolerated, the quartic correction poses severe restrictions to the correct performance of the gate that are not easy to satisfy on atom chips. Thus, for a correct performance, the atoms have to be forced to a given dynamics.

The variant of Ref. [44] to the original proposal [38] can be regarded as the first attempt towards a realistic implementation of the collisional phase gate on an atom-chip device. It employs the hyperfine qubit states \( |0 \rangle \equiv |F = 1, m_F = -1 \rangle \) and \( |1 \rangle \equiv |F = 2, m_F = 1 \rangle \) of \(^{87}\text{Rb}\) whose favorable coherence properties were already discussed in Sec. [1A]. Moreover, its key ingredient, the coherent manipulation of these states with a state-dependent trapping potential and the control of collisions, was realized in recent experiments with BECs [24, 35]. Let us analyze the features of this scheme (see Fig. [9]). The state-dependent potential is split into

\[
V_k(r, t) = u_c(r) + \lambda(t) u_k(r),
\]

where \( u_c(r) \) is a common part and \( u_k(r) \) a qubit-state dependent part \((k = 0, 1)\). The common part of the potential is a time-independent double well potential along \( x \) that can be realized by a static magnetic potential, which is nearly identical for the chosen qubit states. As in Ref. [38], the dynamics can be reduced to a 1D assuming a tight confinement in the transverse dimensions \( y, z \). The state-dependent part can be realized by a microwave near-field potential (see below). It is modulated with a function \( \lambda(t) \), with \( 0 \leq \lambda(t) \leq 1 \). At times \( t < 0 \), when the gate is in its initial state, we have \( \lambda(t) = 0 \) and the atoms are subject to \( u_c(r) \) only. Each atom is prepared in the motional ground of one of the wells of the double well potential. During the time \( 0 \leq t \leq \tau_g, \lambda(t) \neq 0 \) and the potential is state-dependent. The effect of \( u_k(r) \) is twofold: \( u_1(r) \) removes the barrier of the double well for state \( |1 \rangle \) and in this state start to oscillate; the potential \( u_0(r) \) shifts the minima of the double well for state \( |0 \rangle \) further apart in the \( x \)-direction [see Fig. [9]], whereas in the original proposal those atoms do not experience any trap change. In this way, unwanted collisions (atoms in state \( |01 \rangle \)) which are a major source of infidelity, are strongly reduced and the map [2] is implemented.

The state-dependent potential can be realized with microwave near-fields with a frequency near the hyperfine splitting of \(^{87}\text{Rb}\) of 6.8 GHz. Unlike the optical potentials created by non-resonant laser beams, which can be tightly focussed due to their short wavelength, the centimeter wavelength \( \lambda_{mic} \) of microwave radiation poses severe limitations on far-field traps. On atom chips, however, the atoms are trapped at distances \( d < \lambda_{mic} \) from the chip surface, and therefore they can be manipulated by microwave signals in on-chip transmission lines. In
the near field of the source currents and voltages, the microwave fields have the same position dependence as the static fields created by equivalent stationary sources. The maximum field gradients depend on the size of the transmission line conductors and on the distance \( r \), not on \( \lambda_{\text{mw}} \). Therefore, state-dependent microwave potentials varying on the micrometer scale can be realized \([26,46]\).

In a related way, radio frequency fields can be used to generate near-field potentials \([17]\).

When we consider the hyperfine levels \( |F, m_F\rangle \) of the \( 5S_{1/2} \) ground state of a \( ^{87}\)Rb atom, the magnetic component of the microwave field \( \mathbf{B}_{\text{mw}}(\mathbf{r}) \cos(\omega t) \) couples the \( |1, m_1\rangle \) to the \( |2, m_2\rangle \) sublevels, with Rabi frequencies

\[
\Omega_{1,1}^{m,m}(r) = \frac{2, m_2, \mathbf{B}_r(1, m_1)}{\hbar},
\]

for the different transitions (in the rotating-wave approximation). In Eq. \( 5 \), \( \mathbf{B}_r = \mu g_1 \mathbf{J} \) is the operator of the electron magnetic moment \( (g_J \approx 2) \). In a combined static magnetic and microwave trap, as considered here, both the static field \( \mathbf{B}_s(\mathbf{r}) \) and the microwave field \( \mathbf{B}_{\text{mw}}(\mathbf{r}) \) vary with position. This leads to a position-dependent microwave coupling with in general all polarization components present.

The detuning of the microwave from the resonance of the transition \( |1, m_1\rangle \rightarrow |2, m_2\rangle \) is:

\[
\Delta_{1,1}^{m,m}(r) = \Delta_0 - \frac{\mu_B}{2\hbar} (m_2 + m_1) \mathbf{B}_s(\mathbf{r}),
\]

As desired, the potentials for \( F = 1 \) and \( F = 2 \) have opposite signs, leading to a differential potential for the qubit states \( |0\rangle \equiv |1, -1\rangle \) and \( |1\rangle \equiv |2, 1\rangle \).

In addition to the magnetic microwave field, the electric field \( \mathbf{E}_{\text{mw}}(\mathbf{r}) \cos(\omega t + \varphi) \) also leads to energy shifts. By averaging over the fast oscillation of the microwave at frequency \( \omega \), which is much faster than the atomic motion, the electric field leads to a time-averaged quadratic Stark shift. Hence, the total microwave potential for state \( |0\rangle \), \( u_0(\mathbf{r}) \) in \((4)\), is

\[
u_0(\mathbf{r}) = -\frac{\alpha}{4} \mathbf{E}_{\text{mw}}(\mathbf{r})^2 + \frac{\hbar}{4} \sum_{m_2 = -2}^0 \frac{[\Omega_{1,1}^{m,m}(r)]^2}{\Delta_{1,1}^{m,m}(r)},
\]

while the microwave potential for state \( |1\rangle \) is

\[
u_1(\mathbf{r}) = -\frac{\alpha}{4} \mathbf{E}_{\text{mw}}(\mathbf{r})^2 - \frac{\hbar}{4} \sum_{m_1 = 0}^{+1} \frac{[\Omega_{1,1}^{m,m}(r)]^2}{\Delta_{1,1}^{m,m}(r)}.
\]

The atom chip layout shown in Fig. 3 allows one to realize the desired state-selective potential. It consists of two layers of gold metallization on a high resistivity silicon substrate, separated by a thin dielectric insulation layer. The wires carry stationary (DC) currents, which, when combined with appropriate stationary and homogeneous magnetic bias fields, create the state-independent potential \( u_s(\mathbf{r}) \). In addition to carrying DC currents, the three wires on the upper gold layer form a coplanar waveguide (CPW) for a microwave at frequency \( \omega \), which is possible by the use of bias injection circuits. The microwave fields guided by these conductors create the state-dependent potential \( u_s(\mathbf{r}) \).

In order to speed up the correct gate performance, optimal control techniques \([45]\) have been employed. To introduce the related concepts, let us consider a system governed by the time dependent Hamiltonian \( \hat{H}(t, \lambda) \), where \( \lambda \) is the control parameter. Our goal in general is to reach, in a fixed time \( \tau_g \) and for a given initial condition \( |\psi_0\rangle \) at time \( t = 0 \), a certain target state \( |\psi_T\rangle \) with high fidelity. Several iterative algorithms exist that can yield a systematic improvement in the gate fidelity. Here the one developed by Krotov \([49,50]\) has been used. The quantum optimal control algorithm works as follows:

1. an initial guess \( \lambda^{(0)}(t) \) is chosen for the control parameter.
2. the initial state \( |\psi_0\rangle \) is evolved in time according to the Schrödinger equation \( |\psi_\lambda(t)\rangle = U(\lambda, \tau_g)|\psi_0\rangle \) until time \( \tau_g \).
3. an auxiliary state \( |\chi_\lambda(\tau_g)\rangle \equiv |\psi_T\rangle \langle \psi_T | \chi_\lambda(\tau_g) \rangle \) is defined, which can be interpreted as the part of \( |\psi_\lambda(\tau_g)\rangle \) that has reached the objective \( |\psi_T\rangle \); the auxiliary state is evolved backwards in time until \( t = 0 \).
4. \( |\chi_\lambda(t)\rangle \) and \( |\psi_\lambda(t)\rangle \) are propagated again forward in time, while the control parameter
is updated $\lambda^{(j+1)}(t) = \lambda^{(j)}(t) + 2/\eta(t) \cdot \Im \left( \langle \lambda \rangle \frac{\partial \hat{H}}{\partial \lambda} | \psi^{(j+1)}(t) \rangle \right)$, where $j$ refers to the $j$-th iteration of the algorithm. The weight function $\eta(t)$ constrains the initial and final values of the control parameter.

5. steps 3. and 4. are repeated until the desired value of the fidelity is obtained.

Making use of this technique, a gate operation time $\tau_g = 1.11$ ms with a fidelity $F = 0.996$ can be obtained (see also Fig. 4, as shown in Ref. [44], the control parameters being the electrical microwave current injected in the CPW and the radial frequency $\omega_\perp$ through the stationary electrical currents in the wires displayed in Fig. 3 a). We emphasize that with this $\tau_g$ and the long coherence lifetime of the qubit pair chosen, thousands of gate operations can be accomplished. The fidelity calculation includes the effect of several error sources: trap losses and decoherence due to the chip surface, undesired two-photon transitions induced by the microwave, mixing of the hyperfine levels due to the microwave coupling, and qubit dephasing due to technical noise. In the limit of large microwave detuning, the admixture of other states with different magnetic moments to the qubit states is strongly reduced. A last important point is related to the difficulty to prepare the atoms in the vibrational ground state with close to 100% efficiency. This effect, modeled by a finite temperature, has been also included in the analysis. For temperatures $T \leq 20$ nK in the initial double well trap, the fidelity is not reduced significantly [44].

B. Motional-state qubits

Based again on the conditional phase shifts induced by the collision between cold atoms, a number of proposals rely on the manipulation of quantum information stored in motional degrees of freedom. The original proposals [13, 14, 51] dealt with optical lattices, but those schemes can also be implemented using microscopic potentials on chips. Besides magnetic, microwave, or radio frequency traps, chip-based optical traps are of interest in this context. By illuminating a 2D array of refractive or diffractive micro lenses with laser light, a 2D set of diffraction limited laser foci can be formed. Atoms can be confined in the optical dipole potentials generated by the laser foci [52]. In a first experiment, arrays with more than 80 sites were loaded with ensembles of about 1000 trapped $^{85}$Rb atoms in the centre of the 2D configuration and about 100 at the edges [53]. Theoretical proposals for two-qubit gates in this system rely again upon the spatial overlap of two qubits out of initially separated locations. This can be accomplished by illuminating the array of micro lenses with two laser beams with a finite relative angle of propagation creating two interleaved sets of dipole traps [52]. The variation of the relative angle yields a variation in the mutual distance between the trap sets or, alternatively, by using a programmable and computer controllable nematic liquid-crystal spatial light modulator, the trap separation can be varied by changing the periodicity of the modulator [54]. An important feature of these optical micropotentials is the relatively large separation of neighbouring sites ($\sim 125$ µm) which enables individual addressing [55]. In a recent experiment the same group has demonstrated that transport, reloading, and a full shift register cycle ($\sim 55$µm) can be performed with negligible atom loss, heating, or additional dephasing or decoherence [55]. This proves that such a technology is scalable to complex and versatile 2D architectures such that quantum information processing, quantum simulation, and multi-particle entanglement become accessible.

In the quantum gate scheme of Ref. [51], a double well potential contains one atom per well. The logic states $|0\rangle$ and $|1\rangle$ are identified with the single particle ground and excited states of each well, respectively. Initially the barrier is sufficiently high that tunneling between the lowest four eigenstates of a single trapped atom is negligible. When the barrier is lowered in such a way that the single particle excited states (the qubit states $|1\rangle$) of the potential do overlap, tunneling takes place and the energy shift due to the atom-atom interaction increases exponentially. The interaction lasts for a time sufficient to accumulate the required phase shift for a phase gate and subsequently the initial trapping configuration is restored by increasing

Figure 4. Dynamics during the gate operation, shown for $N = 3$ oscillations [44]. The gate time is $\tau_g = 1.11$ ms. Both $\lambda(t)$ and $\omega_\perp(t)$ are used as control parameters. a) Optimal control of the microwave power. Upper plot: initial trial function $\lambda^{(0)}(t)$ (dashed line) and optimized control parameter $\lambda(t)$ (solid line). Each triangular ramp of $\lambda(t)$ corresponds to a full oscillation of state $|\psi_1\rangle$. Lower plot: the difference $\delta \lambda(t) = \lambda(t) - \lambda^{(0)}(t)$ shows small modulations. b) Optimal control of the effective one-dimensional interaction strength via modulation of the transverse trap frequency $\omega_\perp$. c) Evolution of the overlap fidelities during the gate operation: $F_{00}(t)$ (dashed line), $F_{11}(t) = F_{01}(t)$ (dotted line), and $F_{12}(t)$ (solid line), where $F_{ij}(t) = |\langle \psi_{ij}(x_1, x_2, t) | \psi(x_1, x_2, 0) \rangle|^2$ with $\psi_{ij}(x_1, x_2, t)$ being the two particle state. d) Evolution of the gate phase $\phi_g(t)$. The phase shift steps are due to the six collisions in state $|11\rangle$. Copyright (2006) by The American Physical Society.
the barrier again. An accurate use of quantum interference between two-particle states yields an optimised gate duration of 38 ms with an infidelity $F \approx 6.3 \times 10^{-6}$. In the proposal of Ref. [13] the scenario is very similar and it uses the same qubit set. While in Ref. [51] the two-qubit gate is physically realised by lowering and increasing the barrier of the double well potential, in Ref. [13] the (initially) separated traps adiabatically approach (or separate from) each other. In that way it is possible to obtain $\tau_g \sim 20$ ms for a VSWAP two-qubit gate.

The proposal of Refs. [13, 14] uses again motional states, but not strictly the vibrational states of the trap. In the scheme each qubit consists of two separated traps and a single atom. Now, the computational basis $\{ |0\rangle, |1\rangle \}$ is formed in this way: the ground state of the left trap represents $|0\rangle \equiv |0\rangle_L$, whereas the ground state of the right trap represents $|1\rangle \equiv |0\rangle_R$. One- and two-qubit quantum gates are performed by adiabatically approaching the trapping potentials and allowing for tunneling to take place. We note that in such a scheme four wells are needed to implement a two-qubit gate, either arranged in a 1D configuration with the traps on a line or side-by-side in a 2D configuration. Taking into account the different error sources present in this scheme, like fluctuations of the trap positions, photon scattering, and heating, one obtains an error rate of about 0.02, with a single-qubit operation time of 4 ms, and $\tau_g \sim 10$ ms for a two-qubit operation such as a phase gate. Even though the error rate is rather large, the scheme offers several advantages: 1) decoherence due to spontaneous emission reduces the fidelity only marginally; 2) no momentum transfer is effected for single and two-qubit gates; 3) a state-dependent interaction is not required for the implementation of two-qubit gates; 4) the readout is done with a laser beam focused onto one trap minimum and detecting the fluorescence light; 5) since one- and two-qubit gates are realized using the same technique, i.e., by approaching the traps adiabatically, the complexity of the experimental setup would be reduced.

Both of these schemes can be implemented on a chip by means of a combination of static and microwave fields, with the need of trapping only one hyperfine level. However, one can combine the nice coherence properties of the qubit states $|F = 2, m_F = 1\rangle$ and $|F = 1, m_F = -1\rangle$ of the ground state of $^{87}$Rb, and the entanglement produced by cold collisions via the motional states $(|g\rangle, |e\rangle)$. In Ref. [15] two different ways of realizing this concept have been proposed: (a) duplicate the logical state of the storage levels in the motional levels, where $|1\rangle \leftrightarrow |e\rangle$; (b) swap the logical states of the two degrees of freedom, $|g\rangle \leftrightarrow |e\rangle$. Here we consider only the swap scheme.

Given the initial state

$$\frac{\phi_0}{\phi_0} = (a|00\rangle + b|10\rangle + c|11\rangle + d|11\rangle)|gg\rangle,$$  \hspace{1cm} (10)

the swap scheme takes place in three steps:

1. we selectively excite the operation state and de-excite the storage states $\frac{\phi_1}{\phi_1} = \frac{\phi_0}{\phi_0}$,

2. the operation states get a dynamical phase $\phi_2: |\phi_2\rangle = (a|00\rangle + b|ge\rangle + c|eg\rangle + d|ee\rangle)$ through collisions;

3. we swap again the storage and operation states $|\phi_3\rangle = (a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle)|gg\rangle$.

Such a swap gate scheme is not restricted to internal and external degrees of freedom of cold atoms, but it can be applied to any system with at least two degrees of freedom. A selective excitation of vibrational states is required when cold atoms are employed. In order to realize it, the use of two-photon Raman transitions has been suggested. The experimental implementation of such transitions with $^{87}$Rb atoms is rather delicate and a careful analysis is given in Ref. [16]. In a static version of the swap scheme, where the barrier is fixed and it is designed in such a way that the left and right single particle excited states overlap (see also Fig. 5), an operation time for a phase gate of 16.25 ms with a gate fidelity $F > 0.99$ has been predicted [15]. In an optimized version of the gate dynamics, where the barrier is lowered and increased in order to get faster operation times for a desired value of infidelity, it has been possible to achieve fidelities of 0.99 in 6.3 ms and of 0.999 in 10.3 ms [16].

VI. OPTICAL LATTICE BASED SCHEMES

In this section we want to discuss the use of optical lattices for quantum computing, how the lattice potentials can be moved in a state-selective way for implementing the two-qubit gate of Refs. [56] and how these potentials...
can be realized on a chip. Beside this, we shall describe other QIP implementations with optical lattices.

A. Hamiltonian for a degenerate quantum Bose gas in an optical lattice

We assume a Bose-Einstein condensate of atoms in the internal state \( |0\rangle \) to be loaded into a potential \( V_{\text{opt}}(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}) \), where \( V_{\text{opt}}(\mathbf{r}) = \sum_{j=x,y,z} V_j \sin^2(\kappa j) \) is a periodic optical lattice potential and \( V_{\text{ext}}(\mathbf{r}) \) is an additional external potential slowly varying in space compared to \( V_{\text{opt}}(\mathbf{r}) \). Here \( \kappa \) is the wave number of the lasers producing the lattice potential. The many-body Hamiltonian in second quantization reads as Eq. (1), but the sums reduce only to the \( k = 0 \) contribution, with the substitution \( V_k \rightarrow V_{\text{opt}} + V_{\text{ext}} - \mu \), where \( \mu \) is the chemical potential. Expanding the field operators in the Wannier basis (while keeping only the dominant terms), Eq. (1) reduces to the Bose-Hubbard Hamiltonian [57]

\[
\hat{H} = -J \sum_j \hat{b}_j^\dagger \hat{b}_j + \sum_j (E_j - \mu) \hat{n}_j + U/2 \sum_j \hat{n}_j(\hat{n}_j - 1),
\]

(11)

where \( \hat{n}_j = \hat{b}_j^\dagger \hat{b}_j \) counts the number of bosonic atoms at lattice site \( j \) (\( [\hat{b}_j, \hat{b}_k^\dagger] = \delta_{j,k} \)), \( J \) is the tunnelling matrix element, \( U \) describes the (repulsive) interaction between particles at the same lattice site, and \( E_j \equiv V_{\text{opt}}(\mathbf{r}_j) \) is the value of the slowly varying superlattice potential at site \( j \). The ratio \( U/J \) is controlled by the depth of the optical lattice potential \( V_j \). Increasing \( V_j \) (via the intensity of the trapping lasers) reduces the tunnelling matrix element \( J \) and increases the repulsive interaction between the atoms \( U \) [57].

In order to perform gate operations in optical lattices we have to be able to selectively fill each lattice site with exactly one particle. This can be achieved by making use of the phase transition from a superfluid BEC to a Mott insulator (MI) at low temperatures (experimentally demonstrated in Ref. [58]), which can be induced by increasing the ratio of the onsite interaction \( U \) to the tunnelling matrix element \( J \) predicted by the Bose-Hubbard model [59] 60. In the MI phase the density \( \rho_j \) (occupation number per site) is pinned at an integer \( \alpha \in \mathbb{N} \) (when starting from a commensurate filling of the lattice), and thus represents an optical crystal with diagonal long range order with period imposed by the laser light. Particle number fluctuations are thereby drastically reduced and thus the number of particles per lattice site is fixed. The number of particles per lattice site depends on the chemical potential in the isotropic case \( E_j = 0 \) [59], whereas in the non-isotropic case we may view \( \mu - E_j \) as a local chemical potential. Hence, \( \rho_j \) can be controlled by the external potential. Indeed, the repulsive interaction between the particles increases as the optical potential is made deeper. At the same time the hopping rate at which particles move from one site to the next decreases. If the optical lattice is turned on with a time scale much slower than the hopping rate and if the thermal energy \( k_B T \) (\( k_B \) being the Boltzmann constant) can be kept much smaller than the interaction energy between two particles in one site, one can achieve a filling of the optical lattice with exactly one particle per lattice site [57].

Finally, we note that, recently, by means of quantum optimal control, a significant reduction of the preparation time of a MI state with high fidelity has been demonstrated [61] (up to hundreds times shorter than in current experiments). Alternatively, by using the dependence of the interaction energy on the vibrational states occupied by the atoms, the entropy of the MI state can be also drastically reduced as well as the time for the state preparation [62].

B. State selective moving potentials

Following Ref. [50], let us consider alkali atoms with a nuclear spin equal to 3/2 (\( ^{87}\text{Rb}, \ ^{23}\text{Na} \)) trapped by standing waves in three dimensions and thus confined by the potential \( V_{\text{opt}} \). The internal states of interest are hyperfine levels corresponding to the ground state \( S_{1/2} \) as shown in Fig. 6b. Along the \( z \) axis, the standing waves are in a configuration such that two linearly polarized counter-propagating traveling waves with the electric fields \( \mathcal{E}_{1,2} \) form an angle \( 2\theta \) [63], as shown in Fig. 7.

The total electric field is a superposition of right and left circularly polarized standing waves \( (\sigma^\pm) \) which can be shifted with respect to each other by changing \( \theta \),

\[
\mathcal{E}(z,t) = \mathcal{E}_0 e^{-i\omega t} [\mathcal{E}_+ \sin(\kappa z + \theta) + \mathcal{E}_- \sin(\kappa z - \theta)],
\]

(12)

where \( \mathcal{E}_\pm \) denote unit right and left circular polarization vectors, \( \kappa = \nu/c \) is the laser wave vector and \( \mathcal{E}_0 \)
the amplitude. The lasers are tuned between the \( P_{1/2} \) and \( P_{3/2} \) levels so that the dynamical polarizabilities \( \alpha_{\pm} \) of the two fine structure \( S_{1/2} \) states, corresponding to \( m_s = \pm 1/2 \) due to the laser polarization \( \sigma^{\pm} \), vanish, whereas the dynamical polarizabilities \( \alpha_{\pm \pm} \) due to the laser polarization \( \sigma^{\pm \pm} \) are identical [see Fig. 6]. Such a configuration can be achieved by tuning the lasers between the \( P_{3/2} \) and \( P_{1/2} \) fine state levels so that the ac-Stark shifts of these two levels cancel each other. The optical potentials for these two states are

\[
V_{m_s = \pm 1/2}(z, \theta) = \alpha_{\pm} |E_0|^2 \sin^2(az \pm \theta).
\]

For instance, if \( |0\rangle \equiv |F = 1, m_F = 1 \rangle \) and \( |1\rangle \equiv |F = 2, m_F = 2 \rangle \), then the potentials for these hyperfine levels are

\[
\begin{align*}
V_0(z, \theta) &= \frac{1}{4} \left[ V_{m_s = 1/2}(z, \theta) + 3V_{m_s = -1/2}(z, \theta) \right], \\
V_1(z, \theta) &= V_{m_s = 1/2}(z, \theta).
\end{align*}
\]

By using such potentials the atoms can be moved along the \( z \) axis in a state-dependent manner and the gate scheme proposed in Ref. [56] can be implemented. In this proposal, at time \( t = 0 \) the atom \( \alpha \) in the logical state \( |k\rangle \) experiences the potential \( V_{\alpha}^{(k)}(r, t) = V(r^{(k)} + \delta r^{(k)}(t) - r) \), which is initially \( (t < 0) \) centred at position \( r^{(k)} \). The centres of the potentials move according to the trajectories \( \delta r^{(k)}(t) \) with the condition \( \delta r^{(k)}(0) = \delta r^{(k)}(\tau_s) = 0 \), and such that the first atom collides with the second one if and only if they are in the logical states \( |0\rangle \) and \( |1\rangle \). Such state-dependent potentials can be also realized with magnetic microtrap lattices [65, 66], and with state-dependent microwave potentials. The latter can be achieved by using a microwave state dressing scheme where only state \( |0\rangle \) effectively couples to the microwaves, as e.g. in the experiment of Ref. [26].

However, optical lattices can be also realized on a chip. Indeed, the results of Ref. [67] show that it is possible to realize 1D and 2D optical lattices, where the traps are the nodes of the evanescent wave field above an optical waveguide resulting from the interference of different waveguide modes. With a laser power of \( \sim 1 \) mW it is possible to produce tight traps, 150 nm above the on-chip waveguide surface, with trap frequencies on the order of 1 MHz, and with a spatial periodicity of about 1 \( \mu \)m. Moreover, the individual qubits are readily addressable, and it is possible to move 1D arrays of qubits by adjusting the phases of the waveguide modes. The drawback of such technology is that to get strong con-
and trapping techniques for such a scheme are essentially the same as the ones previously presented, and it is also well suited for chip implementations.

D. Optimal atomic transport in optical potentials

In the above outlined quantum gate schemes, based on the fact that the atomic wave functions must be made to overlap, a crucial element is their transport from one site of the optical potential to another one, where the interaction among two atoms takes place. This goal has to be achieved with a very high efficiency. In Ref. [69] it has been showed that the optimized control sequences allow transport faster and with significantly larger fidelity than with processes based on adiabatic transport. This shows again, as we discussed in Sec. V A, the great potential afforded by the toolbox of quantum optimal control for the achievement of high-fidelity quantum computation.

In the experiment described in Ref. [69], a 3D optical lattice has been generated by superimposing, say in the z direction, a 1D optical potential to a 2D independent optical lattice in the x − y plane. This horizontal lattice can be dynamically transformed between single-well and double-well configurations, depending on three controllable parameters: (i) the depth of the potential wells; (ii) the ratio of vertical to horizontal electric field components; (iii) the phase shift \( \theta_b \) between vertical and horizontal light components.

The assumed theoretical 1D model (in the axial direction) is such that the optical potential can be separated along the three spatial directions. This allows to express the atomic wave functions as a product of three independent terms. Additionally, like for the collisional gate dimensionality conditions discussed in Sec. V A, it has been assumed that in the radial confinement the atoms always occupy the lowest vibrational state. In Fig. 11 the overlaps \( f_n^a \equiv p_n(T) = |\langle \phi_n(T)|\hat{U}(T)|\psi_n \rangle|^2 \) of the energy eigenstates \( \phi_n \) of the final potential with the evolved state \( |\psi_n \rangle \) are displayed. Here \( a = L, R \) indicates the initial well occupancy of the double-well potential, whereas \( \hat{U}(T) \) is the single-particle time-evolution operator from time \( t = 0 \) to the final time \( T \). Importantly, the experimental data and the theoretical model are in satisfactory agreement, which proves the accuracy of the theoretical modeling. In addition, both the theory and the experiment show a strong dependence on \( \theta_b \) for the transport of the atom starting in the left site of the double well.

On the other hand, in Fig. 11 the evolution of the single particle probability density is shown. As the figure shows, the optimal time evolution is much less smooth than the adiabatic one, since it takes advantage of quantum interference between nonadiabatic excitation paths to obtain better results. Furthermore, an analysis of the effect of atom-atom interactions on the transport process shows that the optimal control parameter sequences found in the noninteracting case, as the one of Fig. 11, still work when including interaction. Indeed, it has been possible to obtain the same transformation as in the case of the adiabatic transport with a better fidelity and in a time shorter by more than a factor of 3, which represents a relevant improvement in terms of scalability of the number of gates that can be performed before the system decoheres due to the coupling to its environment.

We also mention, that very recently other schemes for moving atoms in optical lattices has been proposed and that the topic has been reinvigorated by the recent experimental achievements on the realization of single qubit rotations [32], on the single site addressability [33, 34], and on the single atom detection [70, 71], as we also discussed in Sec. V B. For instance, one can use optical tweezers, as discussed in Sec. V B, to transport atomic qubits around the lattice and merge them into single lattice sites in order to implement collisional quantum gates [72] or, by...
using alkaline-earth(-like) atoms, the $^1S_0$ ground states and the very long-lived $^3P_0$ excited states can be manipulated completely independently by laser light, allowing the construction of independent optical lattices for the two states \[12\].

Finally, we underscore that the quantum computing models discussed above for optical lattice implementations require state-dependent moving potentials and that the entanglement among qubits is produced by means of collisions between ultracold atoms. However, we would like to mention that, alternatively, the entanglement between trapped atoms in optical lattices can be achieved through the laser-induced coherent electric dipole-dipole interaction of pairs of atoms that are made to occupy the same well \[73\]. Such an approach has two main advantages: neutral atoms are weakly coupled to the external environment, thus the detrimental effects of decoherence are strongly suppressed, and operations can be performed in parallel on a large atomic ensemble, which enables massive entanglement production.

VII. OTHER QUANTUM COMPUTATION MODELS

A. Cavity QED based schemes

Recent experimental advances in cavity QED on a chip have yielded results that promise the full integration and scalability of such cavities. Microscopic Fabry-Perot cavities whose open structure gives access to the central part of the cavity field have been developed. In such cavities strong coupling between a single atom and the cavity mode has been obtained \[74\]. In these experiments a BEC was employed, which can be located deterministically everywhere in the cavity and positioned entirely within a single antinode of the standing-wave cavity mode field. This gives rise to a controlled and tunable coupling rate.

On the theoretical side, proposals for a quantum computer based on a cavity QED model have been put forward. The scheme of Ref. \[75\] assumes $N$ atoms coupled to a single quantized mode of a high finesse cavity. Quantum operations (e.g., a controlled-NOT gate) are realised via the coupling of the atoms with individual lasers and their entanglement is mediated by the exchange of a single cavity photon. In a similar setup a controlled-NOT gate can be performed through a sequence of (destructive) measurements on the atoms and quantum non-demolition measurements of the atom number \[76\]. Because of the randomness of the measurement outcome in
this case the gate operation is probabilistic. Nevertheless, this scheme is more robust against decoherence and cavity losses than the one of Ref. [75]: while in that proposal the infidelity scales as $1/\sqrt{2C_0}$, in Ref. [76] it scales as $\log(2C_0)/2C_0$, where $C_0$ is the cooperativity parameter.

B. Rydberg and ensemble based schemes

Based on such experimental achievements, schemes that exploit the interaction of atoms excited to low-lying Rydberg states [17, 77, 78] are also an appealing solution for QIP with neutral particles. An appropriate sequence of laser pulses above a waveguide can excite the qubits into Rydberg states and entangle them via electric dipole-dipole interactions [67] and by triggering electromagnetically induced transparency in the atomic ensemble it is also possible to transfer atoms between internal states [79]. While the phase gate model suggested in Ref. [17] relies only on the strong dipole-dipole interaction, in another recent proposal [80] one can combine the Rydberg blockade mechanism, recently observed for two atoms [81, 82], with the rapid laser pulse sequence of the well-known stimulated Raman adiabatic passage (STIRAP). This combination with the engineering of a time-dependent relative phase $\phi_R(t)$ between the Rabi frequencies of the two STIRAP laser pulses affords a higher degree of control of the phase of Eq. (2) through the manipulation of geometrical phases. We briefly mention that recently the first demonstration of a CNOT gate between two individually addressed neutral atoms by means of the Rydberg blockade interaction with an experimental gate fidelity of about 0.72 and $\pi$ pulse times of $\sim 750$ ns has been demonstrated [83].

A very recent theoretical analysis [84] shows that not only the interaction strength among the qubits is a limiting factor for the gate operation time, but for resonant excitation, the interaction between two atoms causes a coupling between electronic and nuclear dynamics. This induces vibrational excitation which can be carried away by the laser pulse only if the target state is fully resolved. Hence, the excitation of atoms into Rydberg states yields an interaction that one might expect to allow for nanosecond to sub-nanosecond gate operation times [17], but since the motional state of the atoms needs to be restored at the end of the gate, gates with sub-nanosecond operation time seem difficult to realize.

So far, we discussed only qubits that are represented by individual two-level systems. This kind of qubits requires high control and addressability of individual particles, which raise important challenges for experimentalists. Some theoretical investigations, however, use a symmetric collective state of a mesoscopic atomic ensemble [19], where only one excitation is present in the system. The dipole excitation blockade mechanism of Rydberg atoms works in that direction, because it prevents multiple excitations in an ensemble. The same mechanism used to implement a fast phase gate with two Rydberg atoms can be extended to qubits stored in few-μm-spaced atomic clouds, where each atomic ensemble is a qubit. Alternatively, collective states in ensembles of multilevel quantum systems can be used to store the information [20]. Quantum operations such as one- and two-bit gates are then implemented by collective internal state transitions taking place in the presence of an excitation blockade mechanism, such as the one provided by the Rydberg blockade. For more details on QIP with Rydberg atoms we refer to Ref. [85].

C. Polar molecules based schemes

Up to now, we discussed schemes based on the manipulation of single or ensembles of trapped atoms, but a quite interesting solution to the construction of a quantum computer of large scale is given by the use of polar molecules [86]. Indeed, they incorporate two important features of neutral atoms and ions: long coherence times and strong interactions. Besides this, polar molecules have stable internal states that can be controlled by electrostatic fields. This controllability is due to their rotational degree of freedom in combination with the asymmetry of their structure. By applying moderate laboratory electric fields, rotational states with transition frequencies in the microwave range can be mixed, and the molecules acquire large dipole moments, which are the key property that makes them effective qubits in a quantum processing system. Furthermore, the application of electric field gradients leads to large mechanical forces, allowing to trap the molecules. For instance, the electrostatic Z-trap for polar molecules proposed in Ref. [7] creates a non-zero electric field minimum in close proximity to the surface, analogous to Ioffe-Pritchard type magnetic traps for neutral atoms.

In the pioneer proposal by DeMille [86], qubits are represented by rotational states of a diatomic polar molecule and the coupling among qubits is realized by means of the electric dipole-dipole interaction, which can be also produced by using Raman transitions between scattering and bound states of heteronuclear molecules trapped in optical lattices [57]. The integration of a 1D optical lattice with a superimposed crossed dipole trap allows to confine polar molecules in sites spaced by $\lambda/2$. Such a scheme allows to confine in a trap of length $5 \, \text{mm}$ about $10^4$ qubits for a laser wavelength $\lambda \sim 1 \, \mu\text{m}$ and beam waist of $50 \, \mu\text{m}$ with moderate decoherence rates. Without an external electric field, however, polar molecules have no net dipole moment, and therefore the application of an external electric field is required, which mixes the rotational states. For weak fields the mixing state that arises from the $J = 0$ ($J = 1$, $m_J = 0$) state corresponds to a dipolar charge distribution along (against) the external homogeneous electric field. The logical state $|0\rangle$ ($|1\rangle$) corresponds to the dipole moment oriented along (against) the external electric field. Moreover, the addition of an electric field gradient allows the addressing of
individual molecules. By a proper choice of electric field strengths it is possible to realize, with KCs molecules, a CNOT gate in a time of about 50 µs, thereby enabling about $10^6$ quantum operations within the decoherence time of about 5 s, whose main source is photon scattering from the trap laser [86]. The readout of the computation can be accomplished by state-selective, resonant multiphoton ionization and imaging detection of the resulting ions and electrons or, alternatively, with nearby single-electron transistors [88], which allow to detect the molecular dipole fields.

The above outlined estimates are quite encouraging, but the analysis does not take into account, for instance, the effects caused by the motional states of the molecules, which may induce an additional gate fidelity loss, or the hyperfine structure of the molecules, which makes the initialization of the quantum computation and the operation of quantum gates more complicated. Another source of decoherence for such a scheme arises from the interaction of non-nearest-neighbor qubits, which cannot be switched off locally. The negative effects of such interaction can be removed by using a refocusing (spin-echo) technique, similar to the one adopted in nuclear magnetic resonance quantum computation [11], or, alternatively, by using heteronuclear molecules, which have a different dipole moments for different electronic, vibrational or rotational states and zero expectation value for the dipole moment in the $N = 0$ rotational state ($N$ represents the quantum number of the angular momentum $\mathbf{N}$ of the nuclei of the molecule). This approach allows to make the dipole-dipole interaction “switchable”, therefore making the experimental realization of two-qubit quantum gates less complicated as well as minimizing decoherence. With this method it has been shown that up to $10^6$ gate operations are obtainable within the coherence times, for instance, of NaCl or CaF molecules [89]. Another way to switch on and off the dipole interaction is given by the use of Raman transitions, which transfer the qubit state from a set of non-interacting levels, used for the storage of information, to a set of interacting levels, which allow the qubits to interact. Entanglement can then be yielded by single optical pulses of relatively short duration (i.e., larger than 200 ps) thus allowing for relatively short gate operation times ($\simeq 10 \mu s$ − 1 ms) [90]. Instead, by using vibrationally excited (non-polar) molecules, like acetylene ($\text{C}_2\text{H}_2$), entanglement of two qubits via molecular bindings can be (theoretically) performed, by using optimal shaped femtosecond laser pulses in the infrared regime, even on the picosecond timescale [91].

D. Hybrid QIP implementations

In this section we briefly describe some hybrid QIP schemes, namely combinations of solid-state and atomic qubits in a single quantum processor, as we outlined in the introduction of the paper. The proposals of Refs. [3, 7, 22, 23, 92, 93] suggest to use superconducting wires or superconducting microwave cavities to ‘wire up’ several atomic qubits or to couple atomic qubits to a Cooper pair box on the chip surface, as we briefly described in the introduction. Most of the schemes consider polar molecules [5, 7, 23, 94] as atomic system, but other quantum memories can be realized by Rydberg atoms [92], atomic ions [93], ground state neutral atoms [22], and electron spin ensembles [24]. Hereafter we discuss only the schemes based on polar molecules.

The proposals of Refs. [3, 23] suggest a quantum computer model where ensembles of cold molecules are used as a stable quantum memory by means of collective spin states, whereas a Cooper pair box, connected to the molecular ensemble via a stripline cavity, is used to perform one- and two-qubit operations and readout (see also Fig. 2). In Ref. [3] the ground state and a symmetric collective state with only one excitation present in the ensemble are the qubit states, and therefore an ensemble of molecules carries only two logic states. On the other hand, Ref. [23] proposes a ‘holographic’ memory consisting of $N$ molecules in a lattice, initially all in the same internal quantum state $|g\rangle$ [see Fig. 12(b)]. In this case the quantum information in an incident weak field $\Omega_1 e^{i\mathbf{k}_1 \cdot \mathbf{x}}$, by means of a control field $\Omega_2(t) e^{i\mathbf{k}_2 \cdot \mathbf{x}}$ and the Hamiltonian

$$\hat{H}_q = \sum_{j=1}^{N} \Omega_1 e^{i\mathbf{k}_1 \cdot \mathbf{x}_j} |e\rangle_j \langle g| + \Omega_2 e^{i\mathbf{k}_2 \cdot \mathbf{x}_j} |e\rangle_j \langle f| + \text{h.c.},$$

is transferred onto a collective matter-light excitation which propagates slowly through the medium and is brought to a complete stop by turning off $\Omega_2(t)$.

The coupling in Eq. 14 can be used to map a single-photon state to the collective phase pattern state $|f, q\rangle \equiv 1/\sqrt{N} \sum_j e^{i\mathbf{q} \cdot \mathbf{x}_j} |g_1, \ldots, f_j, \ldots, g_N\rangle$, where $q = k_1 - k_2$ is the wave number difference of the two fields. The set of collective excitations $\{|f, q_s\rangle : s = 1, \ldots, K\}$ can be used to simultaneously encode up to hundreds of qubits in just one sample by associating the logical state $|b_1 b_2 \ldots b_K\rangle$ ($b_i = 0, 1$) with the collective state $|f, q_s\rangle$. Addressing

Figure 12. (Color online). (a) By varying the direction of a control field $\Omega_2(t) e^{i\mathbf{k}_2 \cdot \mathbf{x}}$, an incident single photon with wave vector $\mathbf{k}_1$ may be transferred to different collective storage modes with wave vector $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_2$. (b) The levels $|g\rangle$ and $|f\rangle$ are coupled by a two photon process leaving no population in the electronically excited state $|e\rangle$ (adapted from Ref. [23]). Copyright (2008) by The American Physical Society.
different qubits is then accomplished by applying laser beams from different directions such that the orthogonality condition \( \langle f, q_s | f, q_s \rangle \) is approximately fulfilled (i.e., \( \approx \delta_{f_i q_s} \)), as illustrated in Fig. 12(a). This way of encoding does not pose special problems for atom-chip-like devices, where usually single-atom addressing with laser beams is required.

Finally, we briefly mention, that the hybrid system “atom-molecule” also provides an interesting solution for fast and robust quantum computation [95]. An optical lattice with two different atomic species per site, like \(^{87}\text{Rb}\) and \(^{7}\text{Li}\), forms the quantum register. The quantum information is again stored in hyperfine levels of one neutral atom while the other atom is in a state stable against collisions, such that at ultralow temperatures the scattering of the two atomic species is elastic, thus preventing atom loss and qubit decoherence. Two-qubit operations, like the phase gate, are then accomplished by converting pairs of atoms at two lattice sites into stable molecules with a large dipole moment. The produced molecules can then interact via strong dipole-dipole interactions, therefore resulting in fast quantum gates as discussed in Sec. VII C. Such a system can be also utilized for investigating the generation of many-body entanglement and new Hubbard Hamiltonians [96]. Alternatively, one can use the interaction between a Rydberg atom and a polar molecule in order to realize quantum operations between two molecular qubits [97]. A polar molecule within the electron state in a Rydberg atom can either shift the Rydberg state or produce a Rydberg molecule in a state-dependent manner, resulting in molecular state dependent van der Waals or dipole-dipole interaction between Rydberg atoms.

VIII. CONCLUSIONS AND OUTLOOK

We have reviewed a broad range of theoretical proposals for implementing quantum gates with neutral particles and how they can be realized on a chip. Several of these proposals have been worked out in detail, including investigations of various kinds of imperfections such as decoherence due to atom-surface interactions. High-fidelity quantum gates compatible with the requirements for fault-tolerant QIP seem experimentally feasible even in the presence of these imperfections.

On the experimental side, impressive progress was made in the chip-based coherent control of ultracold atoms. Coherent manipulation of long-lived hyperfine qubit states was demonstrated close to a chip surface [10], and coherent control of motional states is routinely achieved in chip-based atom interferometers [26, 30, 37]. Chip-based lattices were created [66] which could store a large register of qubits. The experimental achievement of single-atom preparation and detection on an atom chip with a fidelity exceeding 99.92% [98] represent important milestones on the way to atom chip based QIP. Another important milestone is the on-chip manipulation of ultracold atoms with an internal-state dependent potential [26], a key ingredient of collisional quantum gates. In addition to this, the recent achievement of the fluorescence imaging of strongly interacting bosonic Mott insulators in an optical lattice with single-atom and single-site resolution [70] strengthens the possibility to effectively realize optical lattice based QIP schemes, as we discussed in Sec. VI. In optical lattice experiments the fidelity for the identification of atoms at a given lattice site is about 98% [71].

With these results, all individual elements for the chip-based two-qubit gate of Refs. [38, 44] have now been demonstrated experimentally. An important challenge for the near future is to combine them in a single experiment. In the related context of quantum metrology with atomic ensembles, a recent experiment has already demonstrated the generation of entangled atomic states on an atom chip [45], using techniques similar to the ones proposed for the quantum gate of Refs. [38, 44].

While the development of chip-based near-field traps was pioneered for ultracold neutral atoms, it has already triggered similar developments for other systems such as ions or molecules. As trapped ions are currently one of the frontrunners in the field of QIP, the recent demonstration of chip-based ion traps is particularly promising [99, 102] as well as the strong coupling between an ion Coulomb crystal and a single mode cavity field [103].

We would like to conclude by briefly mentioning one of the most promising directions of future research for QIP. Indeed, a particularly attractive feature of chip traps is the possibility to combine atomic or molecular qubits with solid-state qubits on the chip surface [3, 7, 22, 23]. Such hybrid systems would combine fast processing in the solid-state with long coherence times for information storage in the atomic system. An impressive degree of coherent control has been demonstrated e.g. for qubits based on superconducting circuits [25, 104-106]. Coherent dynamics as well as decoherence in these systems typically occur on a time scale of nanoseconds to microseconds, several orders of magnitude faster than in atomic gases. A very promising approach to couple atomic and superconducting qubits is the use of superconducting microwave resonators [3, 7, 22, 23]. To combine the necessary cryogenic technology with atom chips represents an experimental challenge which is currently pursued in several experiments.

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