Toffoli gate based on three-body fine-state changing Förster resonance in Rydberg atoms

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We have developed an improved scheme of a three-qubit Toffoli gate based on fine-state changing three-body Stark-tuned Rydberg interaction. This scheme is a substantial improvement of our previous proposal, published in [I.I.Beterov et al., Physical Review A 98, 042704 (2018)]. Due to the use of a different type of three-body Förster resonance we substantially simplified the scheme of laser excitation and phase dynamics of collective three-body states. This new type of Förster resonance exists only in three-body systems, while the two-body resonance is absent. We reduced the sensitivity of the gate fidelity to fluctuations of external electric field and eliminated the necessity to use external magnetic field for fine tuning of the position of the resonance in the electric field scale, compared to the previous scheme of Toffoli gate based on Rydberg atoms. A gate fidelity of 98.5% was demonstrated in the calculations.

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I. INTRODUCTION

Recent advances in quantum information with ultracold neutral atoms include demonstration of quantum phases of matter on a large-scale quantum simulator [1], demonstration of high-fidelity entanglement [2, 3, 4] and CNOT gates in atomic arrays with individual addressing [5]. These achievements are based on creation of defect-free arrays of optical dipole traps loaded with single atoms using spatial rearrangement by a movable optical tweezer [6, 7], high-fidelity coherent laser Rydberg excitation of trapped atoms [2, 3] and strong interatomic interaction, resulting in Rydberg blockade [6, 7]. However, the experimentally demonstrated entanglement fidelity is around 99.1% [8], which makes the atomic systems still staying behind the alternative platforms based on superconductors or ultracold ions, where a fidelity above 99.98% has been demonstrated [9].

Of particular interest today is the implementation of controlled three-qubit quantum gates [10], such as the Toffoli gate, the Deutsch gate, the Fredkin gate, etc. Such gates are key components for many important quantum algorithms, notably the Shor’s algorithm [11], quantum error correction [12] and fault-tolerant computation [13]. In addition, these gates greatly facilitate the implementation of quantum computing in large-scale registers.

Although multi-qubit gates can be decomposed into sequences of two-qubit and single-qubit gates, the lack of precision of two-qubit operations rapidly reduces the fidelity of composite multi-qubit gates [14]. In this regard, we propose to use three-body Förster resonances to implement three-qubit quantum operations. Förster resonance is a special type of dipole-dipole interaction that occurs when the energy levels of the collective states of atoms intersect in an external electric field [12]. Depending on the number of atoms involved in the interaction, they can be either two-body [16] or many-body [17, 18]. A three-body Förster resonance energy transfer (FRET) was first observed for an ensemble of ~ 10^5 cold Cs Rydberg atoms [17]. This type of resonance corresponds to a transition when the three interacting atoms change their states simultaneously. One of the atoms here acts as a mediator of the interaction, carrying away the excess energy. This leads to a Borromean type of the Förster energy transfer, when the ordinary two-body resonance gives a negligible contribution to the population transfer, as the three-body resonance appears at a different dc electric field, with respect to the two-body resonance. It thus represents an effective three-body operator, which can be used to directly implement Rydberg quantum gates.

Previously, we have demonstrated three-body Förster resonances experimentally [19] and proved theoretically that these resonances can be used to implement three-qubit quantum gates [20]. We have also designed a scheme of a high fidelity (> 98%) three-qubit Toffoli gate for neutral atoms, based on the coherent phase dynamics of collective atomic states in the vicinity of such a resonance [21]. However, this scheme was quite complex for experimental implementation due to the need for individual excitation of the atoms into Rydberg states with different principal quantum numbers, as well as for extremely high electric field control precision and for adjustment of the positions of the resonances using an external magnetic field.

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A specific advantage of this scheme is the simplicity of its Toffoli quantum gate based on fine-state changing three-microns.

The dipole-dipole interaction operator between two neighboring atoms located along the quantization axis (Z) can be written as:

\[
V_{dd} = \frac{e^2}{4\pi\varepsilon_0 R^3} (a \cdot b - 3a_z b_z) = -\frac{\sqrt{mc^2}}{4\pi\varepsilon_0 R^3} \sum_{q=-1}^{1} C_{q1-q}^{20} a_q b_{-q}.
\]

Here \(\varepsilon_0\) is the vacuum dielectric constant; \(e\) is the electron charge; \(a\) and \(b\) are the vectorial positions of the Rydberg electrons. This operator couples only two-atom collective states with \(\Delta M = 0\), where \(M\) is the total momentum projection of the collective state. The radial matrix elements of the dipole moment are calculated using a quasiclassical approximation [23].

We consider the interactions of the collective states of three Rb Rydberg atoms \(|n_1l_{j1};(m_{j1}); n_2l_{j2};(m_{j2}); n_3l_{j3};(m_{j3})\rangle\). The Förster energy defect is the difference between the energies of the final and initial collective states. In our recent paper [21], the following scheme of three-body Förster resonance for ultracold Rb atoms was proposed for implementing a Toffoli gate:

\[
|nP_{3/2}; (n + 1) P_{3/2}; (n + 1) P_{3/2} (m)\rangle \rightarrow |nP_{3/2}; (n + 1) S_{1/2}; (n + 1) P_{3/2} (m^*)\rangle
\]

Here \(m\) is the projection of the momentum of the third atom on the Z axis and \(m^*\) is the changed value of this projection. It indicates that the states of all three atoms have been changed. For \(n = 80\) our numeric simulations predicted relatively high fidelity (\(\sim 98\%\)) of the Toffoli gate operation. Nevertheless, the need to initialize atoms into states with different values of the principal quantum number is a significant difficulty for experimental implementation. Other limitations are related to the high sensitivity of the gate to changes in the electric field, as well as the need to use magnetic fields to adjust the positions of resonances. A new scheme of three-body resonances, proposed in [23], is advantageous, since all atoms are initially excited into the same state:

\[
|nP_{3/2}\rangle \otimes^3 \rightarrow |nS_{1/2}; (n + 1) S_{1/2}; nP_{1/2}\rangle
\]
Note that $|nP_{3/2}\rangle^{\otimes 3}$ here denotes the product of three identical ket vectors. In this configuration of three-body interaction, the two-body Förster resonance is known to be absent in rubidium for principal quantum numbers above $n = 38$. Therefore, off-resonant two-body interactions induce small phase shifts but no sizable population transfer, in contrast to the scheme, previously considered in [21]. This substantially simplifies the population and phase dynamics of the collective three-body states, as will be shown below.

The numerically calculated dependences of the collective energy levels involved in three-body Förster resonance, described by Eq. (4) with $n = 70$, on the external electric field are shown in Fig. 1(a) for different fine-structure components of Rb $70P$ state. The intersections with the final quantum state, indicated as 1-4, mark the positions of possible three-body Förster resonances.

Figure 1(b) shows the dependence of the calculated probabilities of the Förster resonant energy transfer on the external electric field when all atoms are initially in the state $|70P_{3/2}(m = 1/2)\rangle$. This corresponds to case (1) in Fig. 1(a). The atoms are located in three individual optical dipole traps along the quantization axis $Z$. The direction of the $Z$ axis coincides with the direction of the external dc electric field. Two resonant features are clearly seen. The splitting and shift of the resonances are caused by multiple channels of three-body Förster interaction through different intermediate quantum states.

### III. THE TOFFOLI GATE

#### A. The gate scheme

The Toffoli quantum gate (or CCNOT gate) is a universal three-qubit quantum gate. It is very important for the effective implementation of many quantum algorithms, in particular, for quantum error correction. This gate can also be represented as a CCZ gate wrapped with Hadamard gates, as shown in Fig. 2(a).

The implementation of the Toffoli quantum gate in a system of neutral atoms was described by Levine et al. in [22]. The proposed implementation is based on a strong blockade of the nearest neighbors in a trimerized 1D array. The achievable gate fidelity in this case was $F = 0.87(4)$(after state preparation and measurement (SPAM) errors correction). These results compare quite well with Toffoli gate implementations with trapped ions ($F = 0.896$ [23]) and superconducting circuits ($F = 0.78$ [20]). However, these values are far from the threshold required for the implementation of fault-tolerant quantum computing in atomic registers ($F \geq 0.99$). Equally important is the fact that quantum gates based on the Rydberg blockade effect require a sufficiently close arrangement of atoms. Förster resonances are one of the promising solutions for working in large-scale registers, where it is required to implement gates between qubits spatially isolated from each other at distances of about 10 microns or more.

The proposed scheme for the implementation of the Toffoli gate is shown in Fig. 2(b). Three Rb atoms are confined in three optical dipole traps located along the direction of the external electric field (Z axis) with interatomic distance $R$. To couple the logical states of qubits (namely, $|0\rangle$ and $|1\rangle$), we propose to use two-photon Ra-

![Diagram](image-url)
man laser pulses that do not populate the intermediate excited state $5P$. An alternative approach based on the use of microwave laser pulses with individual addressing can also be applied. This will require the use of an intense off-resonant laser acting on a selected qubit to ac Stark shift its energy levels into resonance with the microwave radiation [27, 29].

Eight laser pulses are used to implement the gate. As the first step, the pulse 1 is used, which is a $Y$-rotation by $\pi/2$, carrying out the action of the first Hadamard gate. Then, the pulses 2-4 required for the $|1\rangle \rightarrow |70P_{3/2}(1/2)\rangle$ transitions are applied simultaneously to all three qubits. The number in parentheses indicates the projection of the momentum $m_J$ on the Z axis.

In accordance with the proposal [22], we consider the excitation into Rydberg states with the same principal quantum number $n = 70$. This configuration allows us to achieve high fidelity of the quantum gate due to long lifetimes, large dipole moments and coherence of the chosen three-body interaction channels. At the same time, it facilitates the experimental implementation of the scheme, compared to our previous proposal [21].

Depending on the initial state of the system, after laser pulses 2-4, the number of the excited Rydberg atoms varies from zero to three. When all three atoms are excited, the phase of the collective atomic state is shifted by $\pi$, due to the three-body Förster resonance, tuned by an external electric field.

At the final stage, Rydberg atoms are de-excited by laser pulses 5-7. Raman laser or microwave pulse 8 drives the additional $-\pi/2$ rotation of the target qubit around the Y axis, which is equivalent to the second Hadamard gate in Fig. 2(a). The timing diagram of all controlling pulses is shown in Fig. 2(c).

B. Phase and population dynamics

To implement the Toffoli gate, it is necessary to find the conditions under which two- and three-body interactions lead to the required phase shifts of the initially excited collective states. Therefore, it is necessary to optimize the parameters of the atomic system: the interatomic distance $R$, the interaction time $T$ and the value of the external dc electric field. Taking into account the technical limitations of experimental implementations, it is necessary to pay attention to the required accuracy of the parameter values. In particular, we found the following requirements for accuracy thresholds: the interatomic distance must be controlled with an accuracy of 0.1 $\mu$m; the interaction time - 0.01 $\mu$s; the external electric field - $10^{-4}$ V/cm. Here we assume that the maximum allowable deviation of the gate fidelity cannot exceed one percent.

FIG. 3. Numerically calculated time dependences of the population and phase of the initially excited collective states of three interacting atoms. System parameters: (a - f) $R = 10$ $\mu$m; $E = 0.14235$ V/cm; $T = 1.15$ ps; (g - l) $R = 8.5$ $\mu$m; $E = 0.1469$ V/cm; $T = 0.42$ ps.
Figure 3 shows the numerically calculated phase and population dynamics of the initially excited collective two- and three-body Rydberg atomic states for optimized system parameters. Left-hand and right-hand panels of Fig. 3 show the time dependence of the population and phase of initial collective state for interatomic distances $R = 10 \, \mu m$ and $R = 8.5 \, \mu m$, respectively.

If all three atoms are excited into Rydberg states, we observe almost resonant Rabi-like population oscillations (Figs. 3a, g)). In this case, the phase of the state changes by $\pi$ after the interaction time due to the three-body resonances $|70P_{3/2} (m = 1/2)\rangle_{g} \to |70 S_{1/2}; 71 S_{1/2}; 70P_{1/2}\rangle$ (Fig. 3b, h)). This phase shift is sensitive to the electric field which acts directly on the Förster energy defect. It corresponds to the controlled phase shift when all three atoms are in state $|1\rangle$ prior to the Rydberg excitation in Fig. 2(b). Note that Fig. 2(b) shows only one of the possible transition schemes. In the resonant process, we cannot attribute $|70P_{3/2} \to |70 S_{1/2}; 71 S_{1/2}\rangle$ and $|70P_{3/2} \to |70P_{1/2}\rangle$ transitions to a specific atom 1, 2 or 3. The population of initial state after the completion of the interaction is 91.5% due to the finite Rydberg lifetimes and the leakage of population to other collective levels by Rydberg interactions. These are found to be the major sources of the gate error.

Consider the case when only two of the three atoms are in the Rydberg state. Then, due to the selection rule $\Delta M = 0$ only off-resonant two-body interactions $|70P_{3/2} (m = 1/2)\rangle_{g} \leftrightarrow |70 S_{1/2}; 71 S_{1/2} (m = 1/2)\rangle$ are possible. The state $|70S_{1/2}; 71 S_{1/2}\rangle$ can also interact off-resonantly with $|70P_{1/2}\rangle_{g}$ and $|70P_{3/2}; 70P_{1/2}\rangle$ states.

If the atomic ensemble is initially excited to state $|ggg\rangle$ (here $|g\rangle$ is the ground state which can be either $|0\rangle$ or $|1\rangle$, $|g\rangle$ is the Rydberg state), we can consider the influence of the interactions described above on the population and the phase of the final state as negligible (Figs. 3c, d, i, j)). This is due to the fact that two Rydberg atoms are too far apart from each other. According to equation (1), an increase in the distance between atoms by a factor of two causes an eightfold decrease in the strength of the dipole-dipole interaction.

Alternatively, when the ensemble is initially excited into one of the states $|ggr\rangle$ or $|rgg\rangle$, we can observe a significant influence of the off-resonant two-body interactions on the phase of the collective state (Figs. 3e, f, k, l). This leads to the phase shift of the initially excited state, which can be compensated to zero during the interaction time $T$, as shown in Fig. 2(c). This phase shift is found to be sensitive to the external electric field.

Finally, when only one atom in the ensemble is temporarily excited into the Rydberg state, the $\pi$ and $-\pi$ pulses, shown in Fig. 2(b), will return the system into the initial state with zero phase shift. However, temporary Rydberg excitation will result in population loss due to the finite lifetimes of Rydberg states. The trivial case is when no Rydberg atoms are excited. The pulses 2-7 will have no effect in this instance.

In contrast to our previous proposal [21], we obtained the required phase dynamics without the need to use an external magnetic field for fine tuning of the position of three-body Förster resonance in the electric field scale. Moreover, the absence of the two-body Förster resonance in the vicinity of the three-body Förster resonance substantially simplifies the phase dynamics of the collective three-atom states.

### C. Optimization of gate parameters

![Dependence of the fidelity of the Toffoli gate on the dc electric field for two different interatomic distances: $R = 10 \, \mu m$ (red curve) and $R = 8.5 \, \mu m$ (blue curve). The maximum accuracy of 98.5% is achieved with an electric field of 0.14232 V/cm. The interaction times coincide with those indicated in the description of Fig. 3 for both cases. (a) For a wide range of electric field values (0.1-0.2 V/cm). (b) Near the fidelity maxima.](image)

The optimal values of the system parameters were calculated by performing multi-objective optimization using the Nelder-Mead method in order to increase the gate fidelity. As mentioned above, for experimental implementation, these parameters must be controlled with high accuracy. Thus, when developing a gate scheme, it is necessary to take into account all possible sources of the gate fidelity losses arising from insufficient control of parameters and suggest ways to minimize their total effect.

The greatest control accuracy is necessary for the dc electric field: as can be seen from Fig. 1, the resonance peaks are extremely narrow, and even a field variation of $10^{-4}$ V/cm can critically affect the gate fidelity. To mitigate this disadvantage, we propose to reduce the interatomic distances.

Figure 4 shows the dependence of the gate fidelity on the external electric field for two different interatomic distances. It can be seen that with a decrease in distance
the requirements for the accuracy of field value control are significantly reduced. At a distance of $R = 10\ \mu m$, a fidelity loss of 1% (with a maximum fidelity of 98.5%) is obtained for a field mismatch of $10^{-4}\ V/cm$. At $R = 8.5\ \mu m$, the same fidelity loss is obtained only at a field mismatch of about $4 \cdot 10^{-4}\ V/cm$.

It should also be noted that reducing the distance has a positive effect on the timing of the quantum gate. Specifically, the time required for gate implementation is 0.42 $\mu s$ when the distance between atoms is 8.5 $\mu m$. In the case when the interatomic distance is 10 microns, the required time is about 3 times higher.

To estimate the gate fidelity, the method proposed in [30] was used. We considered 6 single-qubit configuration states: $|0\rangle$, $|1\rangle$, $(|0\rangle + |1\rangle)/\sqrt{2}$, $(|0\rangle - |1\rangle)/\sqrt{2}$, $(|0\rangle + i|1\rangle)/\sqrt{2}$ and $(|0\rangle - i|1\rangle)/\sqrt{2}$. We formed a set of three-qubit states as all $6^3 = 216$ combinations of three single-qubit basis states. We simulated the density matrices $\rho_{\text{sim}}$ of all final states after Toffoli gate was applied to each initial state. Then we calculated the fidelity of each final state comparing to the etalon state $\rho_{\text{et}}$, which is the final state of the ensemble after the perfect Toffoli gate is performed [31]:

$$F = \sqrt{\rho_{\text{et}} \rho_{\text{sim}} \rho_{\text{et}}}$$

(4)

Averaging over all 216 states, we calculated the gate fidelity of 98.5%.

**IV. CONCLUSION**

In this paper we proposed a scheme to implement a three-qubit Toffoli gate based on a new type of three-body resonant Förster energy transfer in the ensemble of Rb Rydberg atoms isolated in three individual optical dipole traps. This new type of resonance is based on a change of fine-structure state of one of the atoms involved in the interaction. The collective phase shifts induced by Rydberg interactions are controlled by an external electric field. We have shown that it is possible to reach a fidelity exceeding 98% for a short gate duration form 0.4 $\mu s$ to 1.2 $\mu s$.

Note that in the proposed scheme, off-resonant two-body interactions lead to relatively weak phase dynamics. This reduces the effect of the complex structure of Rydberg energy levels on gate fidelity, which appears to be the major source of gate error if the Rydberg interactions are strong [32]. This also makes it possible to implement quantum gates in large-scale registers (for interatomic distances of $\sim 10\ \mu m$).

Compared to our previous proposal [21], the improved scheme of Toffoli gate is more suitable for experimental implementation, since the initial states of atomic qubits are completely identical. It also does not require the use of a magnetic field to fine-tune the resonance position. In order to minimize the decrease in gate fidelity, we found a compromise between the control accuracies of various experimental parameters (interaction time, interatomic distance and dc electric field value). We managed to achieve a significant reduction in the sensitivity of the circuit to electric field deviations by reducing the interatomic distance, avoiding a decrease in the gate fidelity.

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