Two-qubit controlled-PHASE Rydberg blockade gate protocol for neutral atoms via off-resonant modulated driving within a single pulse

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Neutral atom array serves as an ideal platform to study the quantum logic gates, where intense efforts have been devoted to enhance the two-qubit gate fidelity. We report our recent findings in constructing theoretically a different type of two-qubit controlled-PHASE quantum gate with neutral atoms enabled by Rydberg blockade, which behaves like the hybrid version of the π-gap-π gate and Rydberg dressing gate. Its principle relies upon smooth modulated pulse with specially tailored waveform to gain appropriate phase accumulations for quantum gates while suppressing population leakage error and rotation error. The major features include finishing gate operation within a single pulse, not necessarily requiring individual site addressing, and not sensitive to the exact value of blockade shift. Therefore, we anticipate its fidelity to be reasonably high under realistic considerations for intrinsic errors. Moreover, we hope that such type of protocol may inspire future improvements in quantum gates for other categories of qubit platforms, and that its core ingredients may be helpful in the field of quantum optimal control.

I. INTRODUCTION

Efficient, robust and high-fidelity two-qubit controlled-PHASE gate has become one of the central topics in the research frontier of quantum information with neutral atoms, which is not only important for quantum logic processing [1–3], but also crucial for quantum simulation [4] and quantum metrology [5, 6]. Rydberg blockade [7–10] emerges as one essential tool for this purpose, where the rapid progress in related studies over the past two decades, both theoretical and experimental, has already found many key advances in quantum information science and technology with neutral atoms [2, 3, 10–18]. One prominent feature of neutral atoms is that they behave as not only good candidates for qubit registers, but also good choices for quantum interface with light, where Rydberg blockade is also deemed as helpful [14, 19–28].

So far, many mechanisms of building two-qubit controlled-PHASE gate via Rydberg blockade have been discussed extensively, ever since the gate protocol proposed in the seminal paper of Ref. [29]. For the feasible gate protocols readily compatible with the current atomic physics experimental platforms, when associated with strong blockade shift, it seems to us that they can be approximately divided into four categories.

Category I. Rydberg blockade gate with typical pulse sequence of the so-called π-gap-π, which was introduced as the first example of Rydberg blockade effect’s applications in quantum computing [29]. It attracts persistent theoretical interests and serves as the current mainstream blue print for serious experimental advances. Although it requires individual site addressing, recent progress has suggested that the gate operation can be performed on the order of ∼ 100 ns [30–33].

Category II. Rydberg dressing, whose blueprint was first conceived in the context of quantum gases [34]. The blockade effect can also be explored via Rydberg dressing of the ground state atoms [35, 36], which can in turn yield a two-qubit controlled-PHASE gate protocol [37–38]. Besides its role in the universal quantum computing, Rydberg dressing is suitable for implementing adiabatic quantum computation such as quantum annealing [39], and finds important applications in constructing multi-qubit quantum simulator [40–44]. Meanwhile, essential features of Rydberg dressing serve as an important tool in studying interesting physics of Rydberg anti-blockade phenomena, particularly in atomic ensembles.

Category III. Rydberg anti-blockade gate [41, 42]. Such gate protocols usually requires the exact knowledge of the blockade shift [43], and are practically more sensitive to fluctuations of the relative motion between two atoms.

Category IV. Protocols with simplified pulse sequence but more theoretical compromises, whose fidelity is less than ideal but relatively straightforward to experimentally demonstrate. For example, recently Ref. [44] discussed such a gate protocol with a single square pulse driving ground-Rydberg transition, whose major challenge is that its highest theoretical fidelity limit seems shy for scalable purpose or fault-tolerant quantum computing.
Over the years, intense efforts have been devoted to analyzing theoretically and numerically the performance of Rydberg blockade gate $\pi$–gap–$\pi$ protocols, where both the protocol’s inherent physical limitations and technical imperfections have been taken into consideration. Very often, techniques of adiabatic passage $\pi$, including STIRAP, are employed together with the $\pi$–gap–$\pi$ and Rydberg dressing gate protocols. Tuning the Förster resonance with dc electric fields or microwave have been also anticipated to facilitate gate performance. Nevertheless, experimental fidelities from those two-qubit gate mechanisms seem relatively less optimistic at this moment, despite the overall rapid progress in this field. Therefore, there exists constant push for further explorations in gate protocols following potentially different recipes.

In this article, we report our recent progress in theoretically devising and analyzing a Rydberg blockade type of two-qubit controlled-PHASE gate protocol for neutral atoms via Rydberg blockade, whose working principles rely upon atom-light interaction with a single off-resonant modulated laser pulse driving the ground-Rydberg transition. The modulation of the pulse waveform is engineered such that within the required fidelity, both the control and target atoms will return to original state whether the blockade takes place or not, while gaining the correct phases as required by the two-qubit gate. Approximately speaking, this type of protocol combines the advantages of the $\pi$–gap–$\pi$ gate and Rydberg dressing gates in a hybrid form, while avoiding the $\pi$–gap–$\pi$ gate’s annoying factor of keeping steady population on Rydberg state of control atom during gate operation. Part of the aim is that we hope to translate high-quality ground-Rydberg coherence directly into high-fidelity phase gate.

We anticipate that this protocol is conveniently compatible with the nowadays mainstream experimental platforms. Several major characteristics are worth mentioning here. It may work without individual addressing on the qubit atoms. No microwave is required to drive the Rydberg-Rydberg transitions and henceforth it saves trouble of the complicated microwave electronic equipment and antennas. It does not require the exact knowledge of the magnitude of the Rydberg blockade shift. Its working condition does not involve far off-resonance detuning as that of Rydberg dressing and therefore the gate may be designed to fast operation below 1 $\mu$s with respect to realistic experimental apparatus parameters.

The rest of the article is organized as follows. First we present the basic principles of this two-qubit gate protocol. Then we provide the in-depth performance analysis, including the effect of spontaneous emission, for two different types of modulation. Finally we conclude the article. Some technical details and more explanations for delicate issues are postponed to the supplemental material.

![FIG. 1. Schematic of atomic structure for the Rydberg phase gate under investigation. On the left: the relevant atomic states including the Rydberg blockade between $|r\rangle$ and $|r\rangle$, where the lasers are driving $|0\rangle\leftrightarrow |r\rangle$ on control atom and $|0\rangle\leftrightarrow |r\rangle$ on target atom; on the right: under ideal blockade situation, the linkage pattern for states participating the ground-Rydberg transitions $|01\rangle$, $|10\rangle$ and $|00\rangle$. See Morris-Shore transform at Ref. \cite{53} for a better explanation of comprehending linkage structures. State $|11\rangle$ does not participate the prescribed interactions and stays unchanged through the process. Rydberg states $|r\rangle$ and $|r\rangle$ may be the same or different, depending on the choice of Förster resonance structure. For experimental implementations, typically a bias magnetic field along z will split the Zeeman degeneracy, whose amplitude is assumed to be around a few Gauss to a few tens of Gauss. The Rydberg states $|r\rangle$, $|r\rangle$, $|p\rangle$, $|p\rangle$ will suffer from spontaneous emissions, which is not shown in the diagram.](image1)

II. BASIC MECHANISMS

We first sketch over the basic ingredients, where relevant atomic states of the atom-light interaction are shown in Fig. 1. The qubit basis states of the atoms may be represented by a pair of long-lived hyperfine ground clock states for typical alkali atoms, which can be manipulated by external microwave field or optical stimulated Raman transition. Modulated laser pulses will be applied to drive the ground-Rydberg transitions of the control and target atoms. The consequences of the required operation can be abstracted into two aspects: the boomerang condition that the population returns with unity probability and the antithesis condition that the accumulated phases achieve controlled-Z (C-Z) gate result. When combined with a local Hadamard gate on the target qubit atom ($\pi/2$ rotation for transition $|0\rangle\leftrightarrow |1\rangle$) before and after the controller-PHASE gate, this leads to the universal controlled-NOT gate. If $|r\rangle$, $|r\rangle$ are the same state, then individual atom addressing may not be mandatory and the experiment can be operated through one single laser. For the sake of simplicity in derivations, throughout this article the condition of symmetric driving will be presumed, namely both the con-
control and target atoms will see the same Rabi frequency and detuning in their effective ground-Rydberg transition couplings.

Assuming the presence of ideal Rydberg blockade such that double Rydberg excitation $|rr'\rangle$ is impossible. There are three types of couplings: $|10\rangle \leftrightarrow |1r\rangle$, $|01\rangle \leftrightarrow |r1\rangle$ with Rabi frequency $\Omega_s$ and $|00\rangle \leftrightarrow (|0r\rangle + |0r'\rangle)/\sqrt{2}$ with Rabi frequency $\sqrt{2}\Omega_s$, as can be seen in the linkage structure of Fig. 1. Let $(C_0, C_r)$ denote the wave function for the ground-Rydberg transition of $|10\rangle$ or $|01\rangle$, and let $(X_0, X_r)$ denote the wave function for the ground-Rydberg transition of $|00\rangle$. With these preparations, the problem may be described in the form of a set of equations:

$$
\begin{align}
\frac{i}{\hbar} \frac{d}{dt} \begin{bmatrix} C_0 \\ C_r \end{bmatrix} &= \begin{bmatrix} 0 & 1/2 \Omega_s \\ 1/2 \Omega_s & -\Delta \end{bmatrix} \begin{bmatrix} C_0 \\ C_r \end{bmatrix}; \\
\frac{d}{dt} \begin{bmatrix} X_0 \\ X_r \end{bmatrix} &= \begin{bmatrix} 0 & \sqrt{2}/\Omega_s \\ \sqrt{2}/\Omega_s & -\Delta \end{bmatrix} \begin{bmatrix} X_0 \\ X_r \end{bmatrix};
\end{align}
$$

where the goal is to find appropriate and feasible $\Omega_s$, $\Delta$ to let those relations hold rigidly.

It turns out, such solutions may be acquired, where practically the errand is to find them out and examine their properties. Briefly speaking, our tactics touches upon careful refining efforts for modulations from heuristic approaches. More specifically, first we design waveforms under assumption of perfect adiabatic time evolution process in Eq. (1), and then perform optimizations to suppress the non-adiabaticity effects, where numerical tools serves an essential role in this process. On the other hand, we believe that the accessible solutions aren’t unique and a full characterization remains an open problem.

Except for technical noises, two main types of intrinsic errors exist for our gate protocol: the population leakage error due to spontaneous emission of Rydberg levels during interaction, and the rotation error due to the less than ideal Rydberg blockade with double Rydberg excitation. With properly tailored smooth pulses, the mechanism of adiabatically tracking two-atom dark state gets implicitly triggered under the presence of dipole-dipole exchange interaction $|rr'\rangle \leftrightarrow |pp'\rangle$. Therefore, the rotation error will be suppressed, making the spontaneous emission as the major source of generic error in theory.

### III. WITH BOTH AMPLITUDE AND PHASE MODULATIONS

For $|01\rangle$ and $|10\rangle$, the dynamics amounts to nothing more than a two-level system made from ground-Rydberg transition with time-dependent Rabi frequency $\Omega_s(t)$ and detuning $\Delta(t)$. On the other hand, for $|00\rangle$, its dynamics actually probes the Rydberg dipole-dipole interaction, whose linkage pattern may be summarized as $|00\rangle \leftrightarrow (|0r\rangle + |0r'\rangle)/\sqrt{2} \leftrightarrow |rr'\rangle \leftrightarrow |pp'\rangle$. In order to quantitatively describe the Förster resonance structure of $|rr'\rangle \leftrightarrow |pp'\rangle$, we assume that the coupling strength is $B$ and the small Förster energy penalty term is $\delta_p$ for $|pp'\rangle$. Define the state $|R\rangle = (|0r\rangle + |0r'\rangle)/\sqrt{2}$, the interaction Hamiltonian for this multi-state system is then

$$
H_{I}/\hbar = \sqrt{2}\Omega_s|R\rangle\langle 00| + \sqrt{2}\Omega_s|rr'\rangle\langle R| + B|pp'\rangle\langle rr'| + H.c. + \Delta|R\rangle\langle R| + 2\Delta|rr'\rangle\langle rr'| + \delta_p|pp'\rangle\langle pp'|, \tag{2}
$$

where we have entered rotating wave approximation.

To evaluate fidelity, we first calculate the outcome wave functions from numerically integrating the ODEs. Then, with respect to the four basis two-qubit states $|00\rangle, |01\rangle, |10\rangle, |11\rangle$, we acquire the 4 by 4 transform matrix $U$ representing the functioning of our gate operation. Then the fidelity may be calculated as $F = \langle R| U^\dagger U |R\rangle$.
FIG. 3. More details of the performance of waveforms defined in Eq. (3), for input state $|00\rangle$, averaged over multiple MCWF trajectories. Parameter settings are kept the same as Fig. 2 with the extra considerations for spontaneous emission from Rydberg levels and amplitude fluctuations. The settings are $\gamma_r = \gamma_p = \Omega_n = 2\pi \times 0.1\text{kHz}$. The bottom figure shows that the population return with an error on the order of $\sim 10^{-4}$ after interaction. Apparently, the population of $|rr'\rangle$ remains negligible through the interaction.

$$\left(\text{Tr}(M M^\dagger) + |\text{Tr}(M)|^2\right)/20,$$ where $M = U_{C-Z}^\dagger U$ with $U_{C-Z}$ being the transform matrix of an ideal C-Z gate.

Here, we make the designing goal a little more strict than necessary, such that the population returns with a phase change of 0 for $|01\rangle$ and $|10\rangle$, while the population returns with a phase change of $\pi$ for $|00\rangle$ after interaction. After some refining work on time-dependent adiabatic states [52], we arrive at waveforms described in the following format:

$$\Omega_s(t) = \Omega_0 + \Omega_1 \cos(2\pi t/T_g) + \Omega_2 \sin(\pi t/T_g);$$ (3a)

$$\Delta(t) = \Delta_0 + \Delta_1 \cos(2\pi t/T_g) + \Delta_2 \sin(\pi t/T_g);$$ (3b)

where after optimizations with the respect to the parameters, we have identified a set of values as in Table I.

| $\Omega_0$ | $\Omega_1$ | $\Omega_2$ | $\Delta_0$ | $\Delta_1$ | $\Delta_2$ |
|---|---|---|---|---|---|
| 2.564 | 0.950 | 0.116 | 1.004 | -1.093 | -0.002 |

TABLE I. Sample values for waveforms of Eq. (3) to reach C-Z gate. The unit is $2\pi \times \text{MHz}$, and the gate time $T_g$ is set as 1 $\mu$s.

To demonstrate the actual dynamics, we present the numerical simulation results in Fig. 4, taking the Hamiltonian of Eq. (2) into account. The modulation does not involve unreasonable high frequency components, and the atomic wave function does not go through ‘sudden’ change during the course of gate operation. Note that we have intentionally chosen a symmetric waveform, which makes the visualization better but is not necessary.

Furthermore, with respect to the two types of intrinsic errors, we estimate the influences of spontaneous emission and double Rydberg excitation, particularly for the dynamics associated with input state $|00\rangle$. The numerical evaluation result is shown in Fig. 3 which resorts to quantum jump approach [53, 54], also known Monte-Carlo wave function (MCWF). The decay rate of $|r\rangle$, $|r'\rangle$ and $|p\rangle$ and $|p'\rangle$ are taken as $\gamma_r$, $\gamma_p$ respectively. More-
over, to emulate technical noises such as random fluctuations on the amplitude, we set the Rabi frequency as $\Omega_s(t) + W \cdot \Omega_n$, where $W$ takes random values in each MCWF trajectory uniformly distributed between 0 and 1. A clear signature is that the population in the doubly excited Rydberg state almost all adiabatically returns, thanks to the adiabatic dark state driving mechanism.

### IV. WITH AMPLITUDE MODULATION

![Image of waveform graphs](image)

**FIG. 5.** More details of the performance of waveforms with only amplitude modulation defined in Eq. (4), for input state $|00\rangle$, averaged over multiple MCWF trajectories. Parameter settings are kept the same as Fig. 4, with the extra considerations of $\gamma_r = \gamma_p = \Omega_n = 2\pi \times 0.1\text{kHz}$. Similar to Fig. 3 the population of $|rr\rangle$ remains negligible through the interaction.

For ease of realistic implementations, it is preferred that we only need amplitude modulation, while the pulse starts and ends at zero intensity. We have studied this case and find out that such objective is attainable. Among several candidates, we are particularly interested in the ones of relatively less complexities, such as:

$$\Omega_s(t) = \left(\Omega_0 + \Omega_1(t - \frac{T_g}{2})^2 + \Omega_2|t| - \frac{T_g}{2}|^3\right) \cdot \sin(\pi t / T_g);$$  

$$\Delta(t) = \Delta_0 \equiv \text{constant}.$$  

(4a)  

(4b)

where we purse a symmetric waveform again.

Next, we seek a set of values leading to appropriate phase gate performance. In terms of the phase accumulation for the four basis states, the constraint is:

$$\phi_{11} = \pm \pi - \phi_{00} + \phi_{01} + \phi_{10},$$  

where $\phi_{01} + \phi_{10} - \phi_{00} = \pm \pi$ if $\phi_{11} = 0$.

| $\Omega_0$ | $\Omega_1$ | $\Omega_2$ | $\Delta_0$ |
|----------|-----------|-----------|----------|
| 8.993    | -165.914  | 318.014   | -2.383   |
| $2\pi\times\text{MHz}$ | $2\pi\times\text{MHz}/(\mu\text{s}^2)$ | $2\pi\times\text{MHz}/(\mu\text{s}^3)$ | $2\pi\times\text{MHz}$ |

**TABLE II.** Sample values for waveforms of Eq. (4) to reach a proper phase gate operation. The bottom row shows the units respectively, where the time $t$ is counted in unit of $\mu$s.

After optimization efforts we have reached satisfying results, where a sample set of values is shown in Table II. The corresponding numerical simulation is shown in Fig. 4. It possesses some similarity to Rydberg dressing, where the singly-excited Rydberg state $|R\rangle$ is not heavily populated during the interaction process. The signature of quantum Rabi oscillation seems of less amplitude compared to the case of Fig. 2. From this point of view, the underlying physics mechanism is slightly different between the approach in Section III and this section. Nevertheless, both approaches serve well the purpose of two-qubit phase gate.

We observe that the mechanism of adiabatically tracking the two-atom dark state also plays an essential role here, as can be seen in Fig. 5. The amplitude modulation does not only introduce the correct change in wave function for a phase gate with respect to Eq. (1) and Eq. (5), but also helps to suppress the rotational error. In other words, major limitations on the attainable fidelity are anticipated to mostly come from spontaneous emissions, modulation imperfections and technical noises.

### V. CONCLUSION AND OUTLOOK

When considering the off-resonant driving for the ground-Rydberg transition, we’ve concentrated on the few states that are directly involved in the mechanism. Realistically, the situation is more complicated due to the atom’s many other levels, which may introduce various sources of ac Stark shifts and decoherences [32, 45].

Recent efforts and advances to enhance the fidelity of atom-atom controlled-PHASE gate, including the techniques of utilizing two-atom dark state [33] and smooth driving pulse waveform [32], are also vital and anticipated to offer further improvements to our gate protocol. We are also looking forward to a few other future refinements, including the search for a faster gate operation, further suppression of population leakage, and more user-friendly parameter setting. Stronger robustness against environmental noises in realistic experimental implementations is worth pursuing, where we wish to look for waveforms that are more resilient to technical noises such as amplitude fluctuations. Error correction [57] for our gate
protocol is also part of the long term goal.

For applications with readily available hardware in immediate future, we expect that $\gtrsim 99\%$ fidelity may be obtained for two-qubit gate in 1D, 2D or 3D atomic arrays with a gate time less than 1 µs. The hope is that with experimental platform capable of reaching $>99\%$ fidelity, the neutral atom’s characteristic advantage of scalability will be clearly manifested. In the long run, we hope that the predicted theoretical limit can be reached such that this gate protocol can facilitate the practical quantum information processing capabilities of neutral atom qubits, which we think will take a lot of patience and hard work to tackle all the known or unknown obstacles. Our faith with the Rydberg blockade gate is that high-fidelity ground-Rydberg Rabi oscillation shall be directly translated into high-fidelity controlled-PHASE gate. We also anticipate that our work will help the endeavors for the ensemble qubit approach $^{20, 26, 28}$ and the Rydberg-mediated atom-photon controlled-PHASE gate $^{23, 24, 26, 28}$.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the funding support from the National Key R&D Program of China (under contract Grant No. 2016YFA0301504 and No. 2016YFA0302800) and the fundamental research program fund at ICQI of National University of Defense Technology. The authors also acknowledge the hospitality of Key Laboratory of Quantum Optics and Center of Cold Atom Physics, Shanghai Institute of Optics and Fine Mechanics. The authors gratefully thank the help from Professor Mingsheng Zhan, Professor Liang Liu and Professor Mark Saffman who essentially make this work possible. The authors also thank Professor Xiaodong He and Professor Tian Xia for enlightening discussions.

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