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Robust Rydberg-interaction gates with adiabatic passage

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We show that with adiabatic passage, one can reliably drive two-photon optical transitions between the ground states and interacting Rydberg states in a pair of atoms. For finite Rydberg-interaction strengths an adiabatic pathway towards the doubly Rydberg excited state is identified when a constant detuning is applied with respect to an intermediate optically excited level. The Rydberg interaction among the excited atoms provides a phase that may be used to implement quantum gate operations on atomic ground-state qubits.

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The interaction between atoms excited to high-lying Rydberg states make cold atoms, trapped in tweezer arrays or optical lattices, promising candidates for the implementation of quantum computing [1] and for the study of complex many-body and light-matter problems [2]. In Ref. [1] it was shown that controlled phase operations between two neutral atoms can be performed either when the atoms experience very strong or very weak dipole-dipole (Rydberg) interactions. In the former, so-called Rydberg blockade regime, one excited atom causes a sufficiently large energy shift of Rydberg states in a neighboring atom to effectively detune it away from resonance and block its excitation by a laser field. In the weak interaction regime, both atoms can be excited to Rydberg states and attain a phase due to the weak Rydberg interaction. Two-qubit gates and generation of entanglement have been demonstrated experimentally in the blockade regime [3–5], and the two-atom gate proposals have been followed by a variety of schemes for fast quantum gates with atomic ensembles [6–9], entangled state preparation [10,11], quantum algorithms [12,13], quantum simulators [14], and quantum repeaters [15]. Other schemes using, e.g., the interaction in an antiblockade regime [16] and in conjunction with strong dissipation [17,18], have been proposed.

In this work, we propose a protocol that applies for Rydberg interaction strengths that are too weak to yield the blockade mechanism, yet too strong to be ignored when the atoms are excited with resonant laser fields. This intermediate regime applies to atoms beyond nearest neighbor separation in multiatom architectures [19], and two-qubit gates between such atoms are a prerequisite for effective implementation of algorithms on multiqubit registers. The key ingredient in interaction-based gates is the possibility to reliably excite two atoms to the Rydberg states, and we apply adiabatic passage [20], which is a widely used technique for robust transfer of population between states in atomic and molecular systems [21–23].

We introduce the adiabatic dark states of coherently driven three-level atoms and discuss how they are affected by the interaction between the excited states. We then determine adiabatic eigenstates of the two-atom Hamiltonian and show how a constant detuning of the driving fields can be used to obtain an adiabatic pathway towards the doubly Rydberg excited state. Finally, we include dissipation and atomic motion to estimate gate fidelities and optimal parameters for the gate operation.

We consider atoms with two ground hyperfine states, $|0\rangle$ and $|1\rangle$, and a Rydberg state, $|r\rangle$, which can be excited via the intermediate state $|p\rangle$; see Fig. 1. The atoms experience an energy shift V_R, when both atoms occupy the Rydberg state $|r\rangle$. The transition Rabi frequencies between states $|1\rangle$ and $|p\rangle$ and between $|p\rangle$ and $|r\rangle$ are denoted $\Omega_1(t)$ and $\Omega_2(t)$, respectively, and a detuning Δ may be applied with respect to the intermediate level $|p\rangle$. The Rydberg and optically excited states decay by spontaneous emission of radiation, and we assume that the Rydberg state lifetime is much longer than the optical state lifetime $\gamma_r \ll \gamma_p$. The total Hamiltonian describing the interacting Rydberg atoms is

$$H(t) = H_1 \otimes \mathcal{I} + \mathcal{I} \otimes H_2 + V_R|rr\rangle\langle rr|, \tag{1}$$

with single-atom Hamiltonian operators ($\hbar = 1$),

$$H_j = \Delta|p\rangle_{jj}\langle p| + (\Omega_1(t)|1\rangle_{jj}\langle p| + \Omega_2(t)|p\rangle_{jj}\langle r| + \text{H.c.}), \tag{2}$$

($j = 1,2$). For concreteness, we consider the following time-dependent Rabi frequencies ($0 \leqslant t \leqslant 2\tau$):

$$\Omega_1(t) = \Omega \sin\left(\frac{\pi}{2\tau}t\right)\Omega_2(t) = \Omega\left|\cos\left(\frac{\pi}{2\tau}t\right)\right|. \tag{3}$$

The atoms initially populate the ground atomic states and as long as the adiabatic condition $\Omega\tau \gg 1$ is fulfilled, when $V_R = 0$, the $|1\rangle$ component of both atoms follows the dark state (zero eigenvalue state at any time t), $|D\rangle \equiv \cos\theta|1\rangle - \sin\theta|r\rangle$, $\tan\theta = \Omega_1(t)/\Omega_2(t)$. All the population in the product state $|11\rangle$ is thus transferred to the doubly excited Rydberg state $|rr\rangle$ and back without populating the intermediate level $|p\rangle$ of either of the atoms.

In the limit of strong interaction, i.e., $V_R > \Omega \gg 1/\tau$, the dark-state dynamics is destroyed, resulting in optical excitation and spontaneous decay [22]. At the end of the pulse sequence (3) there is an equal probability of finding either of the atoms in the Rydberg state, while the other atom may have experienced several spontaneous emission events and the coherence and entanglement between the atoms is lost.

In the opposite limit of weak interaction, i.e., $V_R \ll \Omega$, the interaction term in Eq. (1) causes a perturbative energy shift given by the constant V_R multiplied by the $|rr\rangle$ population of the time-dependent dark state $|DD\rangle$, $P_{rr}(t) = \sin^4\theta$. The dark state thus accumulates the corresponding time-dependent phase

$$\phi(t) = V_R \int_0^t P_{rr}(t')dt'. \tag{4}$$

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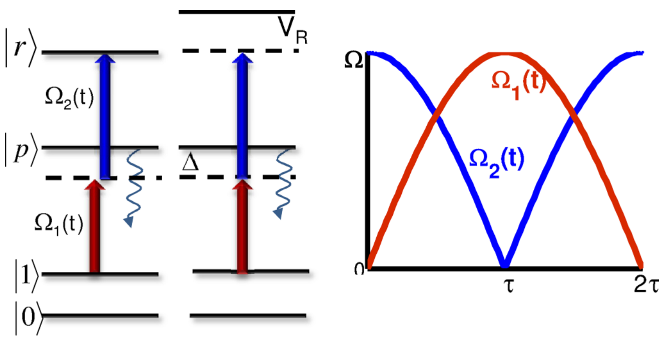

FIG. 1. (Color online) Energy-level diagram of atoms driven by two-photon laser transitions with Rabi frequencies $\Omega_1(t),\Omega_2(t)$ between ground $|1\rangle$ and Rydberg states $|r\rangle$. The pair of Rydberg states experience the interaction V_R. The right-hand side of the figure shows the counterintuitive pulse sequence for the Rabi fields $\Omega_1(t),\Omega_2(t)$, driving the atoms from $|1\rangle$ to $|r\rangle$ and back. This process yields a phase gate on the ground qubit states $|0\rangle$, $|1\rangle$.

In a single cycle of the Rabi frequency evolution (3), the product state $|11\rangle$ attains a phase $3\tau V_R/8$ after time 2τ, while all other states $|10\rangle,|01\rangle,|00\rangle$ do not get this phase as they do not populate the doubly excited state $|rr\rangle$. Thus one achieves a controlled phase gate $U_\phi = \mathcal{I} + (e^{i\phi} - 1)|11\rangle\langle 11|$ and for $\tau = \frac{8\pi}{3V_R}$ we achieve the maximally entangling π-phase gate for two atoms. Since $V_R \ll \Omega$, this gate is slow and thus subject to Rydberg state dephasing and decay.

We are now interested in the intermediate regime, $V_R \sim \Omega$. Here, the interaction term constitutes a non-negligible detuning for the transition to the state $|rr\rangle$, and the atoms populate undesired state components, including the short lived intermediate state, resulting in a loss of gate fidelity. We first analyze the dynamics of the system by solving the unitary dynamics generated by the Hamiltonian given in Eq. (1). This is followed by a master equation analysis of the effects of dissipation.

In Fig. 2 we show the $|rr\rangle$ population, $P_{rr}(t)$ as a function of time $t \in [0,\tau]$ for $V_R = \Omega/2$. The lower, blue (gray) curve in the figure shows the results for a vanishing detuning, $\Delta = 0$, with respect to the intermediate state, and we see that the excitation of two Rydberg atoms is almost completely suppressed. The reason for this can be understood by a closer examination of the adiabatic eigenstates of the Hamiltonian. $|11\rangle$ and $|rr\rangle$ are, indeed, eigenstates at times $t = 0$ and $t = \tau$, respectively, but, they are not adiabatically connected: For $\Delta = 0$, the former state evolves along the interacting two-atom dark state [10]

$$|\psi(\theta)\rangle = \frac{1}{\sqrt{\cos^4\theta + 2\sin^4\theta}}[(\cos^2\theta - \sin^2\theta)|11\rangle - \cos\theta\sin\theta(|1r\rangle + |r1\rangle) + \sin^2\theta|pp\rangle]. \quad (5)$$

Adiabatic following of this state does not populate the doubly excited Rydberg state at $t = \tau(\theta = \pi/2)$, but it populates the $|p\rangle$ state and suffers from spontaneous emission. At $t = \tau$, the state $|rr\rangle$ is instead one of the other eigenstates of the time-dependent Hamiltonian, which adiabatically correlates with a state that populates the doubly excited Rydberg state with a probability of 0.5 for times $t = 0,2\tau$. In Fig. 3(a), for

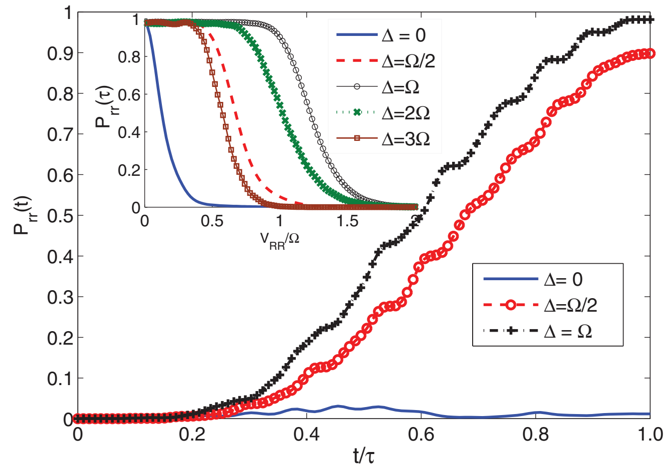

FIG. 2. (Color online) The population of the doubly excited Rydberg state $P_{rr}(\tau)$ is shown as a function of time for fixed $V_R = \Omega/2$ and pulse length $\tau = 0.25\ \mu$s. The different curves correspond to different values of the intermediate state detuning Δ. In the inset we show for different values of Δ how $P_{rr}(t = \tau)$ varies as a function of the Rydberg interaction strength V_R. Both atoms are initially in their ground states, $|\psi(0)\rangle = |11\rangle$, and all calculations assume $\Omega/2\pi = 50$ MHz.

the same parameters as in Fig. 2, we show the eigenenergies of the time-dependent Hamiltonian. The middle (blue [gray]) and the upper (red [gray]) dashed curves show the energies for the two-atom dark state and for the state attaining $|rr\rangle$ at $t = \tau$, respectively. The curves approach each other, and the small population of $|rr\rangle$ in Fig. 2 (lower, blue [gray] curve) is due to nonadiabatic transitions between the adiabatic eigenstates.

The picture changes when we apply a finite detuning from the middle level. This breaks the degeneracy of the states in

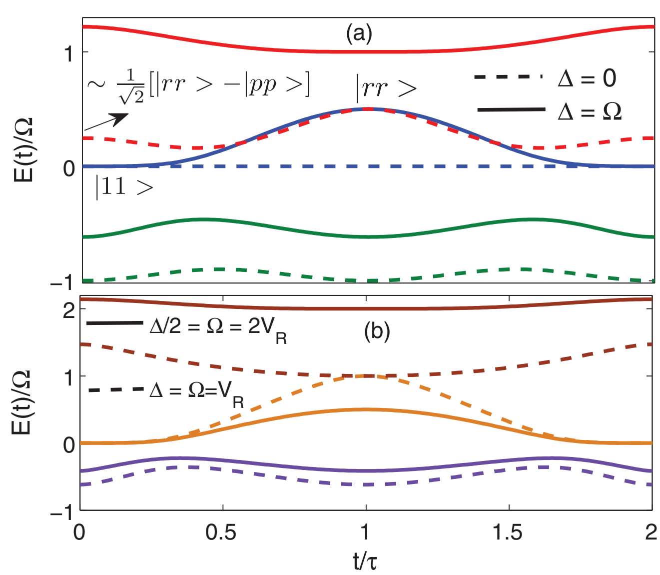

FIG. 3. (Color online) Three energy eigenvalues are shown for the time-dependent Hamiltonian (1): (a) for vanishing Δ (solid lines) and for $\Delta = \Omega = 2V_R$ (dashed lines) and (b) for $\Delta/2 = \Omega = 2V_R$ (solid lines) and for $\Delta = \Omega = V_R$ (dashed lines). The values of Ω and τ are the same as those used in Fig. 1.

Eq. (5), and if the detuning is chosen to be comparable to V_R and Ω, new adiabatic eigenstates are formed with significantly modified character. The solid lines in Fig. 3(a) show the eigenenergies of the time-dependent Hamiltonian for the case $\Delta = \Omega = 2V_R$ and now, indeed, the state $|11\rangle$ *is* adiabatically connected to $|rr\rangle$ along the middle (blue [gray]) solid line. The time-dependent population of the the state $|rr\rangle$ during the time evolution with $\Delta = \Omega = 2V_R$ is shown as the upper, black curve in Fig. 2, and indeed, it reaches a value near unity at $t = \tau$.

Let us now address the conditions for high-fidelity phase gate performance with Δ, Ω, and V_R of comparable magnitudes. Our request for a finite V_R to yield the desired phase evolution is fulfilled if we take $\Omega \sim V_R$ and $\Delta \sim \Omega$. The detuning should not be taken much larger, since that would cause nonadiabatic transfer towards the low-energy eigenstate [lower, violet (gray) solid line in Fig. 3(b)], while making V_R much larger than Ω will cause nonadiabatic transfer towards the high-energy eigenstate [upper, brown (dark gray) dashed line in Fig. 3(b)].

Our calculations show that it is possible to rapidly transfer atoms from $|11\rangle$ to $|rr\rangle$ and back. To ensure adiabaticity, the total time must be long enough, $\Omega\tau \gtrsim 1$. This constraint is similar to the conventional single-atom adiabaticity condition, which must anyway be fulfilled such that the qubit product states $|01(10)\rangle$ evolve adiabatically along $|0D(D0)\rangle$.

Due to the Rydberg interaction and the detuning the adiabatic state leading to the double excitation of the Rydberg state will have a nonzero population in $|p\rangle$ which is subject to the effect of spontaneous emission and decay, and the Rydberg state is also subject to decoherence and decay. To evaluate the dynamics in the presence of these dissipative effects we therefore solve the master equation

$$\partial_t \rho = i[\mathcal{H}_{\text{eff}}, \rho] + \sum_{j,k} \mathcal{C}_k^{(j)^\dagger} \rho \mathcal{C}_k^{(j)}, \tag{6}$$

where $\mathcal{H}_{\text{eff}} = \mathcal{H} - \frac{i}{2}\sum_{j,k} \mathcal{C}_k^{(j)^\dagger}\mathcal{C}_k^{(j)}$, and $\mathcal{C}_k^{(j)}$ are Lindblad operators, which describe the decay processes of the jth atom by spontaneous emission of light, $\mathcal{C}_0^{(j)} = \sqrt{\gamma_0}|0\rangle_{jj}\langle p|, \mathcal{C}_1^{(j)} = \sqrt{\gamma_1}|1\rangle_{jj}\langle p|$ $(\gamma_p = \gamma_0 + \gamma_1)$. Rydberg state decay is described by similar terms, e.g., $\mathcal{C}_r^{(j)} = \sqrt{\gamma_r}|p\rangle_{jj}\langle r|$, but it is a much slower process, and we also consider the dephasing of the Rydberg state $\mathcal{C}_{rd}^{(j)} = \sqrt{\gamma_{rd}}(\mathcal{I} - 2|r\rangle\langle r|)$.

In Fig. 4, we show results where we have solved the master equation for systems starting in a product state $\frac{1}{2}(|0\rangle + |1\rangle)(|0\rangle + |1\rangle)$. We applied $\Delta = \Omega = 2\pi \times 50$ MHz, and for different values of V_R/Ω we adjusted τ to obtain the desired π phase shift. The curve in the figure shows the final-state fidelity when the decay rates are taken as $\gamma_p/2\pi = 6$ MHz, $\gamma_r/2\pi = 1$ kHz, $\gamma_{rd}/2\pi = 10$ kHz, corresponding to realistic parameters for Rb atoms with $|p\rangle = |5P_{3/2}\rangle$ and $|r\rangle$ having principal quantum number $n = 97$ [24]. The fidelity is deteriorated for small values of V_R due to dephasing and decay of the Rydberg states (as $\tau \sim 1/V_R$), while for large values of V_R nonadiabatic processes are important (as $\tau \sim 1/\Omega$). In the inset we show how the population of the state $|rr\rangle$ at the time τ varies as a function of the duration of the adiabatic process. The lower curve is obtained with the same parameters as the main plot, relevant for Rb atoms, while the upper curve is obtained with a decay rate of $\gamma_p/2\pi = 1.01$ MHz corresponding to Cs atoms, with $|p\rangle = |7P_{1/2}\rangle$, and Rydberg states with $n = 100$. The effect of nonadiabaticity can already be seen for $\tau \sim 0.1$ μs, where the double excitation probability becomes oscillatory as the energy difference between close adiabatic eigenstates is of order $1/\tau$. The state transfer is better than 90% for both sets of parameters, and inspection of the parameters show that a duration as short as $\tau = 0.25$ μs leads to the desired π phase shift and a phase gate with acceptable fidelity.

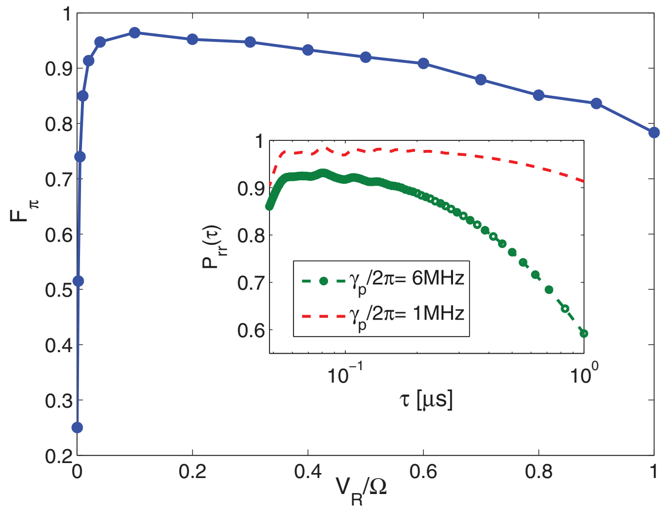

FIG. 4. (Color online) The optimal final-state fidelity for the π-phase gate, $F_\pi \equiv \text{Tr}[U_\pi \rho(0) U_\pi^\dagger \rho(2\tau)]$, applied to atoms initialized in $\rho(0) = |\psi\rangle\langle\psi|$, where $|\psi\rangle = \frac{1}{\sqrt{2}}[|1\rangle + |0\rangle]$, is shown as a function of the Rydberg interaction strength V_R. The decay rates applied in the simulations are $\gamma_p/2\pi = 6$ MHz, $\gamma_r/2\pi = 1$ kHz, $\gamma_{rd}/2\pi = 10$ kHz. In the inset we show the double excitation probability at the end of half cycle (starting in $|11\rangle$), $P_{rr}(\tau)$, as a function of τ for $\gamma_p/2\pi = 1.01$ MHz (red [gray] dashed line) and $\gamma_p/2\pi = 6$ MHz (green [gray] circles). The strength of the interaction and the single-photon Rabi frequency are chosen to be $V_R/2\pi = 25$ MHz and $\Omega/2\pi = 50$ MHz.

Atoms excited to the Rydberg state during the gate experience a force that entangles their motion with the qubit degree of freedom [25] and thus decreases the gate fidelity. We now estimate this loss of fidelity for atoms separated by a distance r, initialized in the ground states of tight harmonic traps with trapping frequency ω_0 and a position uncertainty r_0. For the C_6/r^6 van der Waals interaction, the atoms in $|rr\rangle$ experience a force $\sim\frac{6}{r}V_R$. The amplitude for the harmonic motion to become excited is estimated by first-order perturbation theory, $\sim\frac{6r_0}{2r}\frac{V_R}{\omega_0}(1 - e^{-i\omega_0\tau})$, where the factor $\frac{1}{2}$ takes into account that the force only applies for the $|rr\rangle$ component of the state, with a population varying between zero and unity during the gate. For ^{87}Rb atoms separated by a distance $\sim$11.7 μm and excited to the high-lying Rydberg state ($n = 97$) [24], the Rydberg interaction energy yields $V_R/2\pi = 4$ MHz. With the single-photon Rabi frequency $\Omega/2\pi = 50$ MHz, the duration of the phase gate is $2\tau \sim 0.5$ μs, and if the atoms are held in optical tweezer traps with $\omega_0/2\pi = 36$ kHz and $r_0 = 390$ nm, the probability of excitation to the first excited motional states during the gate time 2τ is then only $\sim$0.02. Using instead an optical lattice to trap the atoms, the motional frequency is much higher and the ground state width is an order of magnitude smaller, and the effects of motional excitation may be ignored.

In conclusion, we have shown that atoms with intermediate value Rydberg interaction strengths, incompatible with the blockade mechanism but too strong to be dealt with by perturbation theory, can be excited reliably by adiabatic passage and accumulate a well-controlled phase, useful for entangling quantum gates. The result may be important for quantum computing architectures, where some but not all atoms are within the blockade radius distance of each other and where different variants of interaction gates may become useful.

The interaction strength in our numerical example is typical for highly excited atoms at intermediate to large separation, and also for closer atoms excited to lower lying Rydberg states. By comparison, it is possible to operate a blockade gate if the Rabi coupling frequency is kept well below the value of V_R. On resonance with the intermediate level that would, however, be subject to decay and a significantly lower fidelity, while for a large detuning Δ, the requirements on laser coupling strengths become severe. Our simulations assumed a Rabi frequency stronger than V_R, and we have investigated the simple interaction gate for the same parameters, i.e., the direct resonant excitation to $|rr\rangle$ with the strong fields. This process, however, also suffers from fidelity loss due to decay from the intermediate optically excited state. The rapid adiabatic process in comparison seems to make optimum use of the robust near-resonant state transfer and the (almost) dark state character of the intermediate states.

If all two-qubit gates have infidelities at the few-percent level, scalable fault-tolerant quantum computing is not possible. In our proposal, the minimal error is found by a competition between nonadiabaticity and dephasing, favoring long and short gate duration, respectively. By increasing the Rabi frequencies one may therefore maintain adiabaticity with a decreased gate time, and there is no fundamental reason that Rabi frequencies higher than the 50 MHz assumed in our calculations should not be available with new laser sources. We further note that the interaction gate proposed here should not replace the conventional high-fidelity blockade gate at short distances. Work on distributed quantum computation, e.g., Ref. [26], is suggestive that fault tolerance may indeed be obtained with quantum information strategies that exploit a combination of high-fidelity local gates and moderate-fidelity gates over intermediate distances.

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