

# Optimal control of Rydberg lattice gases

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We present optimal control protocols to prepare different many-body quantum states of Rydberg atoms in optical lattices. Specifically, we show how to prepare highly ordered many-body ground states, GHZ states as well as some superposition of symmetric excitation number Fock states, that inherit the translational symmetry from the Hamiltonian, within sufficiently short excitation times minimising detrimental decoherence effects. For the GHZ states, we propose a two-step detection protocol to experimentally verify the optimal preparation of the target state based only on standard measurement techniques. Realistic experimental constraints and imperfections are taken into account by our optimisation procedure making it applicable to ongoing experiments.

## I. INTRODUCTION

Quantum simulation and quantum information processing crucially rely on the ability to create precisely controllable multipartite quantum systems, with designed Hamiltonians and low decoherence rates compared to experimental time scales. Ultracold atoms in optical lattices, laser-coupled to high-lying Rydberg states, provide an appealing platform for engineering such quantum systems. Optical potentials trapping the atoms provide highly flexible control over spatial geometries [1, 2], with lattice sites that can be loaded with single atoms with near-unit fidelity [3, 4]. Quantum gas microscopes represent an established technology for observing the quantum state of individual atoms within the lattices [5].

Strong and tunable long-range interactions between atoms across lattice sites can be established by laser-coupling them to Rydberg states, with interaction strengths that can be far in excess of all other energy scales in the system [6, 7]. A striking consequence is the so-called Rydberg blockade [8, 9], which was successfully employed to entangle pairs of atoms [10–12], as well as ensembles of atoms [13–19]. Rydberg-excited atoms in lattice geometries can be described with Ising spin models [20–23], which have recently seen impressive experimental confirmation [19, 24, 25]. Extended spin models can be realised by adding exchange interactions through coupling of multiple Rydberg levels [26–32], or by introducing controlled dissipation [33–40]. Finally, even a general purpose Rydberg quantum simulator [41] and quantum annealer [42] have been proposed.

Evidently, Rydberg atoms hold high promise for applicability in quantum information processing and quantum simulation. Yet, thus far most experimental investigations have been limited to studying *dynamics* of Rydberg-excited systems, while previously predicted interesting ground state physics and associated quantum phase transitions [20–23, 43, 44] remain largely unexplored. The primary limiting factor preventing observation of many-body ground states is the finite lifetime of the Rydberg states [7]. Although Rydberg atoms boast relatively long lifetimes of up to tens of microseconds [45],

it is still a very stringent requirement that the typically complex ground state preparation scheme is executed well before a single decay event occurs. Preliminary experimental success has been achieved in preparing crystalline states of regularly spaced Rydberg excitations in a 1D chain of atoms [46]. These experiments effectively probed the first few steps of a full Devil’s staircase, i.e. the stepwise increase of the Rydberg atom number in the many-body ground state with increasing laser detuning or system size, that characterises the ground state phase diagram of a lattice gas with power-law interactions [47]. The experiment in Ref. [46] employed a carefully designed adiabatic pulse scheme [21, 48–50], slowly evolving the initial ground state with no Rydberg excitations into the desired crystalline state.

An adiabatic state preparation scheme, however, has some inherent limitations. Firstly, it has to be executed slowly compared with the minimum energy gap *by definition*, which is directly at odds with the previously stated necessity of performing the state preparation as fast as possible. Secondly, many-body states that are not adiabatically connected to a trivial initial state are out of reach of adiabatic preparation. To overcome these limitations, we turn to the tools of Optimal Control (OC) [51–55]. Stimulated by earlier successes of OC in quantum information processing [56–62], and the design of many-body quantum dynamics [63–65], as well as the successful applications in experiments [66–69], we adopt the “chopped random basis” (CRAB) and dressed CRAB (dCRAB) optimal control method [64, 70, 71] for quantum state preparation in Rydberg lattice gases. We will showcase three examples: (i) crystalline states of regularly spaced excitations [46], (ii) GHZ states, relevant for quantum information processing tasks [72–76], and (iii) an arbitrary superposition state.

The paper is organized as follows. In Sec. II we provide a description of the Rydberg system under study, as well as an outline of the relevant experimental considerations. Sec. III demonstrates the results for the Rydberg crystalline state preparation and the obtained excitation staircase. In Sec. IV we show the optimized dynamics for creating and detecting a GHZ state which encodes the qubits in groups of

atoms collectively sharing an excitation, complemented by an arbitrary quantum superposition state preparation scheme described in Sec. V. Finally, Sec. VI summarizes the paper and provides an outlook on exploring the so-called quantum speed limit of state preparation in Rydberg atoms.

## II. BASIC DESCRIPTION

The system we consider is composed of a two-dimensional lattice of  $N$  atoms, which can be realized experimentally either in an optical lattice [46, 77] or in an array of optical dipole traps [2], or even in dense disordered gases by targeted laser excitation [78]. Laser light couples the atomic ground state  $|g\rangle$  to a high-lying Rydberg state  $|e\rangle$  with a Rabi frequency  $\Omega$  and frequency detuning  $\Delta$ , as illustrated in Fig. 1(a). Experimentally, such Rydberg state transitions can either be driven by a two-photon transition via a low-lying intermediate state [7] or by a direct single-photon transition [12, 17, 25]. In the present calculations we focus on the specific situation of previous lattice experiments [46, 77] where Rubidium atoms have been excited to  $43S_{1/2}$  Rydberg states via a far detuned intermediate  $5P_{3/2}$  state with two laser beams.

If two atoms at different lattice sites with positions  $\mathbf{r}_i$  and  $\mathbf{r}_j$  are excited to the Rydberg level, they experience strong van der Waals interactions,  $V_{ij} = C_6/|\mathbf{r}_i - \mathbf{r}_j|^6$ . For the selected  $43S$  state the corresponding  $C_6 = 1.625 \times 10^{-60} \text{Jm}^6$  [46, 79]. This system can be described by the Hamiltonian

$$H = \frac{\hbar}{2} \Omega \sum_i (\hat{\sigma}_{eg}^{(i)} + \hat{\sigma}_{ge}^{(i)}) + \sum_{i \neq j} \frac{V_{ij}}{2} \hat{\sigma}_{ee}^{(i)} \hat{\sigma}_{ee}^{(j)} - \hbar \Delta \sum_i \hat{\sigma}_{ee}^{(i)} \quad (1)$$

where the operators  $\hat{\sigma}_{\alpha\beta}^{(i)} = |\alpha_i\rangle\langle\beta_i|$  denote the atomic transition and projection operators for the  $i$ th atom at position  $\mathbf{r}_i$ .

In Fig. 1(c) we show the energy spectrum of the system Hamiltonian (1) in the classical limit  $\Omega = 0$ . In this case, all eigenstates are tensor products of excitation number Fock states on each site, i.e., many-body Fock states corresponding to a given spatial configuration of site-localized Rydberg excitations.

Increasing the laser detuning lowers the energy of the excited atomic state and, therefore, favours the excitation of Rydberg atoms as seen in Fig. 1(c). Therefore, the low-energy sector of the spectrum is composed of ordered Rydberg atom configurations which minimize the total interaction energy [21]. On the contrary, the GHZ state resides in the high energy region of the spectrum where the  $N$ -atom ground state  $|gg \dots g\rangle$  becomes degenerate with the fully excited state  $|ee \dots e\rangle$  [80]. This degeneracy occurs at the critical detuning  $\hbar\Delta_c = N^{-1} \sum_{i < j} V_{ij}$ , marked in Fig. 1(c). At the final time of the GHZ states preparation the detuning is tuned at  $\Delta_c$ .

Accurate pulse shaping of the Rydberg excitation laser provides accurate experimental control of both  $\Omega(t)$  and  $\Delta(t)$ . This permits to steer the many-body quantum dynamics of the atomic lattice and to prepare specific many-body states starting from the simple initial state  $|gg \dots g\rangle$ , with all atoms in their ground state. While the basic idea of this approach [21, 48, 49] has been demonstrated in recent experiments [46, 77], preparation fidelities have remained limited

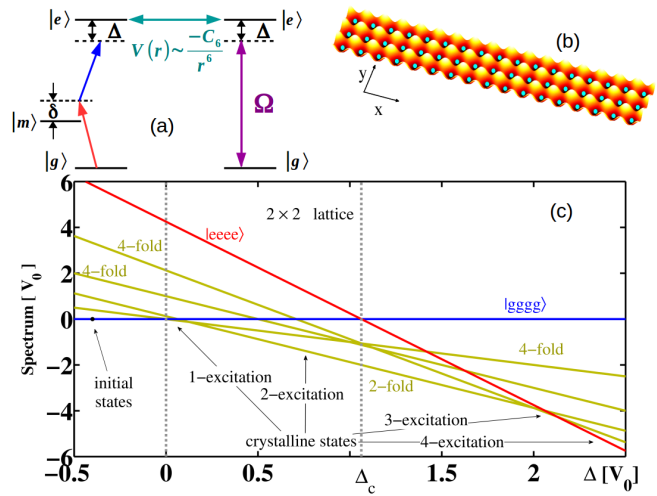


FIG. 1. Rydberg atomic gas. (a) The level scheme of the  $^{87}\text{Rb}$  atom in an optical lattice site. The two-photon process induced by the two control lasers (left) is described by a two-level Rabi model with the coupling  $\Omega$  and the detuning  $\Delta$  (right). (b) The unit-filling optical lattice is tailored into a  $3 \times L$  bar shape. The strong repulsive van der Waals interactions result in the Rydberg blockade effect with a blockade radius approximately  $8a$  such that each group of 3 atoms on the  $y$  axis effectively forms a super-atom. Such a system can be described as a one-dimensional chain along the  $x$  direction with  $\sqrt{3}$  enhanced Rabi coupling. (c) Energy spectrum of a  $2 \times 2$  square lattice in the classical limit ( $\Omega = 0$ ), which is similar to that of a  $3 \times L$  rectangular lattice. The energies of  $|gggg\rangle$  and  $|eeee\rangle$  are highlighted with blue and red, respectively. The low-lying sections of the spectrum for bigger systems are similar to this one. The crystalline state preparation works in the small detuning regime, where the ground state has well-defined total number of excitations that are localized along the lattice sites periodically in space. The states  $|gggg\rangle$  and  $|eeee\rangle$  become resonant at a detuning  $\Delta_c$  (defined in the main text). The dotted gray lines are guidelines for the quantum phase transition point  $\Delta = 0$  and the crossing detuning point  $\Delta_c$ .

by lattice imperfections and unavoidable transitions between the ground state and the low lying excited states. Here, we use optimal control techniques to mitigate such limitations.

We apply the dCRAB method to the preparation of crystalline states, GHZ states as well as an arbitrary superposition state in Rydberg atom lattices. In general the dCRAB method identifies the optimal temporal shapes of the control parameters, which have been expanded on a randomized truncated Fourier basis, through iteratively updating the coefficients of the basis functions using a numerical minimization (e.g. simplex) method, which enables to obtain better fidelities from iteration to iteration. In order to draw a close connection to ongoing experiments, we incorporate typical parameter constraints, limiting the Rabi frequency to  $\Omega/2\pi \leq 400\text{kHz}$  [46, 77], and imposing a truncation on the highest Fourier frequency for synthesising  $\Omega(t)$  and  $\Delta(t)$  at 8.3MHz and 0.5MHz, which translate into a minimum rise and fall time for  $\Omega$  and  $\Delta$  of 60ns and 1000ns, respectively. In this paper, we constrain the maximal amplitude of  $\Delta$  to be 2MHz as in the experiments [46]; however, this cutoff is not a fundamental limit. We will see later that even with this limitation

we can prepare high-fidelity crystalline states and GHZ states, and if we allow for larger detunings  $\Delta$  in the optimization, the results can only improve. Finally, in order to account for lattice defects due to non-unity filling, an ensemble of  $N_r = 50$  realizations of the system each with 10% empty rate for arbitrary sites have been considered in the optimization, where the average fidelity, which is labelled as  $F^C \equiv |\langle \psi^C | \psi(T) \rangle|^2$  and  $F^G \equiv |\langle \psi^G | \psi(T) \rangle|^2$  for crystalline state  $|\psi^C\rangle$  and the GHZ state  $|\psi^G\rangle$ , respectively, is the optimization figure of merit. Here the bars represent the ensemble average over  $N_r$  realizations. Therefore, as we will show, the optimized results are robust against lattice occupation defects.

### III. CRYSTALLINE STATE PREPARATION

In order to prepare a crystalline state with a given number  $n_{\text{ex}}$  of Rydberg excitations, one can drive the system through a sequence of level crossings by chirping the frequency detuning from negative to positive values as shown in Fig. 1(c). Such a near-adiabatic modification of the low-energy many-body states [21, 49, 81] has been demonstrated experimentally in [46]. However, a strictly adiabatic preparation of the absolute ground state is hampered by the finite lifetime of the excited Rydberg atoms, which limits the available evolution times. Consequently, slight crystal defects emerge from unavoidable transitions between the ground state and the low-lying excited many-body Fock states. In [46] the employed excitation pulses allowed to prepare an ordered quantum state of slightly delocalized Rydberg excitations, rather than the actual ground-state crystal consisting of a single Fock state component.

Below we demonstrate theoretically high-fidelity ground state preparation within experimentally relevant preparation times using optimal control. Following the experimental scenario of [46], we consider a quasi-one-dimensional geometry in the form of a  $3 \times L$  lattice as illustrated in Fig. 1(b), where the lattice space  $a = 532\text{nm}$ . Since the transverse extent is considerably smaller than the Rydberg blockade radius, this geometry behaves as a one-dimensional chain of length  $L$  with a collectively enhanced Rabi frequency  $\sqrt{3}\Omega$  [46].

In Fig. 2(a) we show the pulse shape optimised via the dCRAB optimal control method [71] for the generation of a 3-excitation crystal in a chain of length  $L = 17$  for an excitation pulse duration of  $4\mu\text{s}$ . The resulting Rydberg excitation density is nearly identical to that of a perfect three-atom crystal, as shown in Fig. 2(b) where only very weak fluctuations around the optimal Rydberg atom positions occur. The quality of a prepared Rydberg crystalline state has been quantified through the total population of Fock states with given excitation number  $n$ , i.e.,  $P_n \equiv \langle \sum_{i_1, \dots, i_n} |e_{i_1}\rangle \langle e_{i_1}| \otimes \dots \otimes |e_{i_n}\rangle \langle e_{i_n}| \rangle$  [46]. A more stringent evaluation than  $P_n$  is the state fidelity. Our optimal control scheme reaches a high ground state average fidelity over  $N_r$  imperfect realizations of  $F^G > 0.85$  and a high final population  $P_3 = 0.97$  of 3-excitation Fock states. Notice that for this Rydberg lattice gas system the quasi-adiabatic scheme tends to obtain states with low fidelity but relatively high  $P_n$  because of unavoidable transitions to the low-lying

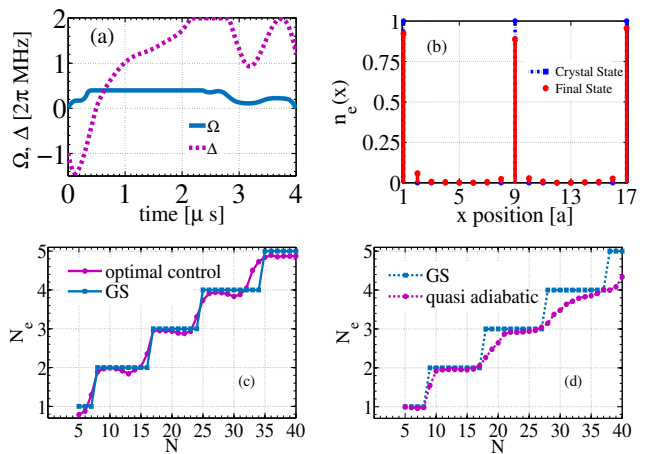


FIG. 2. Rydberg crystalline state preparation. (a) Optimal control driving parameters. (b) Excitation density  $n_e(x) \equiv \langle e_x | \rho | e_x \rangle$  of the 3-excitation crystalline state (blue) and the average final state from dCRAB optimal control (red). The average fidelity  $F^C$  is larger than 0.85. (c,d) Total excitation number staircase as a function of the lattice length for the classical states (blue curves with square markers), i.e., the ground states at final times, and the prepared states (purple curves with circle markers), obtained by applying the pulses from optimal control (c) as well as from the quasi-adiabatic method (d) [82] to systems with different size  $N$ .

excited states, which have displaced excitations with respect to the actual ground state. Here  $n$  is the excitation number of the target crystalline state, and for the current example  $n = 3$ . Even though our protocol is run in an imperfectly prepared lattice with defect, the achieved fidelity yields a significant improvement over previous work, where  $P_3 = 0.91$  could be achieved for an ideal lattice [46]. Note that these numbers can be further increased for higher Rabi frequencies, which are now available for single-photon Rydberg excitation as recently demonstrated in [25].

The enabled high preparation fidelity shows up most prominently in the so-called Rydberg blockade staircase [21]. As Fig. 2(c), our optimised preparation pulse yields sharp transitions between the different excitation numbers  $N_e$  and enables the high-fidelity preparation of ordered Fock states with  $N_e = 5$ . Both features represent significant improvements with respect to the excitation pulses employed in both theory and the experiment of Ref. [46] (also see Fig. 2(d) for the numerical excitation staircase obtained by using the pulse [82] in Ref. [46]).

Fig. 3 illustrates the Rydberg excitation dynamics induced by our optimised laser pulse. As demonstrated by the time evolution of the energy [Fig. 3(a)], energy gap [Fig. 3(b)], the overlap between the instantaneous state and time-local ground state [Fig. 3(c)] as well as the excitation number distribution and the instantaneous state fidelity [Fig. 3(d)], the optimized system dynamics indeed remains near adiabatic and closely follows the instantaneous many-body ground state during the first  $3\mu\text{s}$ . This suggests that adiabatic preparation methods [21, 48, 49] indeed provide a useful strategy for preparing low-energy many-body states [46]. However, the

final stage of the optimised system dynamics significantly deviates from adiabaticity, which ultimately yields the enhanced ground state fidelity described above. Notice that the optimized control pulses presented here are robust against the lattice imperfections arising from non-unity filling of atoms. Incoherence process, e.g. Rydberg state radiative decay, only plays a minor role on a time scale of  $4\mu\text{s}$ , as can be seen from the total decay probability  $P_d(t) \equiv \int_0^t \Gamma N_e(\tau) d\tau$ , where  $N_e(\tau) = \langle \sum_i |e_i\rangle \langle e_i| \rangle$  is the total excitation number of the state at time  $\tau$ , and  $\Gamma = 11.8\text{kHz}$  is the single atom radiative decay rate for the  $43S$  state of  $^{87}\text{Rb}$  [83]. For the optimized evolution the total decay probability at the final time is only  $P_d(T) = 0.1$ .

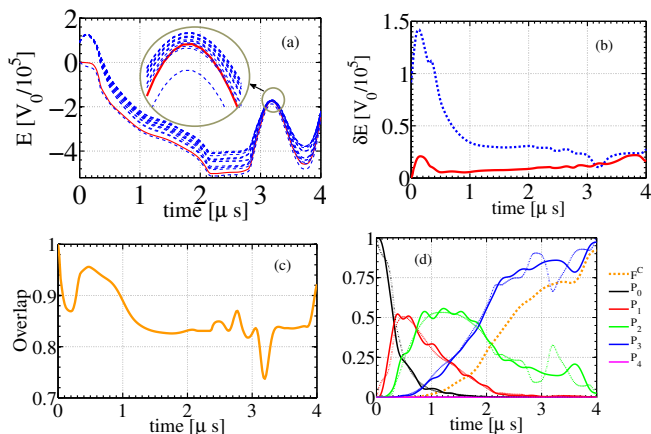


FIG. 3. Dynamics of the Rydberg crystallization. (a) Low-lying energy spectrum (blue dashed curves) and the energy of the instantaneous state from the optimized dynamics (red solid curve). We zoom in at the curves between 3.1 and 3.3  $\mu\text{s}$  in the inset, during which the energy of the optimized dynamics goes into the excited spectrum. (b) The energy gap between the first excited state and ground state (blue dashed curve) as well as the energy difference between the instantaneous state and the ground state (red solid curve). In the time window from 3.1 to 3.3  $\mu\text{s}$  the red curve is above the lowest blue curves, which means the energy of the instantaneous state is higher than the first excited state. (c) The overlap between the instantaneous state  $|\psi(t)\rangle$  and the time-local ground state  $|\psi_G(t)\rangle$ . This overlap measures how close the optimal dynamics is to the adiabatic evolution. (d) Fidelity ( $F^C$ , orange dashed line) and the probability of excitations with given numbers,  $P_n$ , for the instantaneous state (solid curves) and the time-local ground state (dotted curves).

Recent numerical work [50] pointed out that the preparation scheme employed in [46] would yield a rather low ground state fidelity  $F^C \lesssim 0.2$  for the short pulse duration of  $4\mu\text{s}$  used in the experiment [46]. It was, hence, concluded that adiabatic crystal state preparation requires substantially longer excitation times at which dissipative processes would inevitably start to play a significant role [50]. The above results (see Fig. 2 and Fig. 3), however, demonstrate that optimal control allows to alleviate this problem by facilitating high-fidelity ground state preparation for time scales for which the excitation dynamics remains highly coherent.

#### IV. GHZ STATE PREPARATION AND DETECTION

Having demonstrated the power of optimal control techniques for preparing ordered low-energy states of Rydberg excitations, we now consider the high-energy region of the many-body energy spectrum. One area of particular interest lies around  $\Delta_c$ , as marked in Fig. 1(a), where the  $N$ -atom ground state,  $|G\rangle \equiv |g_1, g_2, \dots, g_N\rangle$ , becomes degenerate with the fully excited state  $|E\rangle \equiv |e_1, e_2, \dots, e_N\rangle$ , which allows to generate maximally entangled GHZ states,  $|\psi^G\rangle = (|G\rangle + e^{i\theta}|E\rangle)/\sqrt{2}$  [80].

Due to the strong Rydberg-Rydberg atom interaction the preparation of such high energy states requires a different lattice geometry than that of the previous section. Specifically, we consider an optical lattice with the aforementioned parameters but filled in such a way [84] as to obtain 4 qubits each of which locates at one corner of a  $10 \times 10$  square lattice. In every corner, only  $2 \times 2$  lattice sites are filled with one atom each, in which only one Rydberg excitation can exist and be shared coherently by the  $2 \times 2$  sites because of the blockade effect thus encoding the  $|1\rangle$  state for the qubit. The  $|0\rangle$  state of one qubit corresponds to all its 4 constituent atoms in the ground state. A collection of  $N_{\text{bl}}$  atoms ( $N_{\text{bl}} = 4$  in our example) in a blockade sphere is also called a “superatom”, featuring in addition a collective enhancement of the effective Rabi frequency with a factor of  $\sqrt{N_{\text{bl}}}$  [18, 85–87]. The large qubit spacing ensures a moderate interaction energy of  $\hbar^{-1}C_6/(8a)^6 = 0.4125 \times 2\pi\text{MHz}$  for the  $43S_{1/2}$  Rydberg state used in [46, 77], while the use of multiple adjacent atoms reduces the detrimental effects of lattice defects as described above.

Because of their highly entangled nature, the preparation of GHZ states is much more sensitive to decoherence processes than that of the classical crystalline states discussed in the previous section. In particular, a single Rydberg state decay would completely decohere a prepared GHZ state and project the system onto a separable state. Alleviating such undesired effects once more requires very short operation times, i.e. it calls for optimised preparation pulses.

Fig. 4(a) shows such an optimised pulse for a targeted GHZ state with  $\theta = \pi/2$  and a chosen pulse duration of  $3\mu\text{s}$ . The time evolution of the corresponding fidelity is depicted in Fig. 4(b) and yields a final average value of  $F^G = 0.92$ . Note that such high fidelities are indeed obtained despite a significant fraction of lattice defects around 10%. Remarkably, the fidelity that can be obtained for a defect-free atomic lattice is virtually perfect with  $1 - F = 9 \times 10^{-5}$ . Such conditions and geometries can, for example, be realized with optical dipole-trap arrays as demonstrated in a number of recent experiments [2–4, 19]. As can be seen later, the optimal quantum dynamics differs significantly from the preparation protocol proposed in Ref.[80], where the accessible many-body states are constrained to  $|G\rangle$  and  $|E\rangle$ , and GHZ states are generated by inducing Landau-Zener transitions between them. As shown in Fig. 4(b), the optimised preparation pulses presented here, on the contrary, exploit a significantly larger fraction of the underlying Hilbert space for high-fidelity generation of GHZ states within a short preparation time. Indeed the chosen  $3\mu\text{s}$

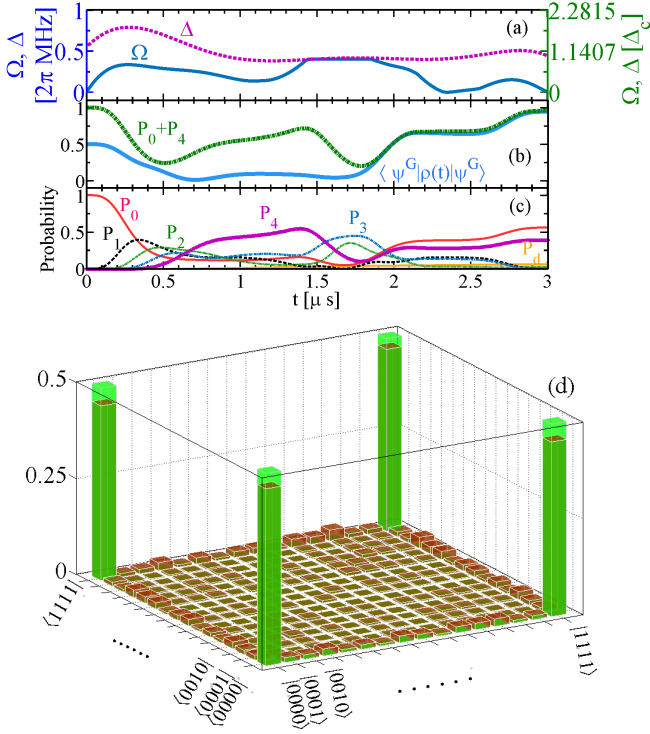


FIG. 4. GHZ state preparation. (a) Optimized control parameters. The detuning  $\Delta$  at the final time has been fixed to be  $\Delta_C$  in Fig. 1, see the right vertical axis. (b) Fidelity for the GHZ state with  $\theta = 0.5\pi$  (cyan solid curve), and population in the subspace spanned by  $|0000\rangle$  and  $|1111\rangle$  (green dotted curve), when applying the optimized control in panel (a) to one realization without lattice defects. The fidelity between the final state of this realization and the GHZ state is approximately 0.94. (c) Probability  $P_n \equiv \langle \sum_{i_1, \dots, i_n} |1_{i_1}\rangle \langle 1_{i_1}| \otimes \dots \otimes |1_{i_n}\rangle \langle 1_{i_n}| \rangle$  of excitations with given numbers  $n$  and the decay probability  $P_d$  for the instantaneous state  $\rho(t)$ . (d) State tomography  $|\langle i_1, i_2, i_3, i_4 | \rho | j_1, j_2, j_3, j_4 \rangle|$  of the average final states (brown) and the GHZ state (green).

preparation time of Fig. 4 is sufficiently short to ensure a total decay probability  $P_d(t)$  of less than 0.07 [see Fig. 4(c)]

The experimental detection method for this system is limited to the excitation probability on each site, which is sufficient to probe the crystalline state [46, 77] but not enough to demonstrate the presence of the GHZ state directly. Here we propose to apply a sequence of measurements to probe GHZ states, exploiting the fact that information on the coherence present in the state can be extracted from the free time evolution of the system [88].

We start from the natural assumption that many copies of identical final states can be obtained simply by repeating the experiment, as is routinely done to improve measurement statistics. The first step is then to perform a standard excitation measurement [46] on many copies of the final states  $|\psi(T)\rangle$ . If the system is in the GHZ state, 50% of the measurement outcomes will result in no excitations while the other 50% will result in 4 excitations. No other configuration should appear for any individual measurement. That shows that the final state (not necessary pure) lives in the subspace spanned

by the states  $|0000\rangle$  and  $|1111\rangle$  as  $\rho_\psi^{\text{sub}} = \begin{pmatrix} 1/2 & \gamma e^{i\alpha} \\ \gamma e^{-i\alpha} & 1/2 \end{pmatrix}$  with  $0 \leq \gamma \leq 1/2$ . Clearly, the GHZ states  $|\psi^G\rangle$  are described by  $\rho_\psi^{\text{sub}}$  for  $\gamma = 1/2$  and  $\alpha = \theta$ .

In the second step, we still need to distinguish between  $|\psi^G\rangle$  and the other states in  $\rho_\psi^{\text{sub}}$ . One intuitive way to distinguish between them is of course to measure the purity of the final state. Recently, the Greiner group has shown an experimental method to probe the purity of the state for cold atoms in an optical lattice through measuring the average parity of the atomic interference between identical two-copy states [89]. However, this parity scheme is not particularly suitable for many-body Rydberg systems, since the long-range interactions between Rydberg atoms from the same copy are difficult to switch off in the interference. Hence, we propose a free-evolution scheme in which one can distinguish them by simply evolving the systems with a detection Hamiltonian  $H_d = \frac{\hbar}{2} \Omega_M \sum_i (\hat{\sigma}_{eg}^{(i)} + \hat{\sigma}_{ge}^{(i)}) + \sum_{i \neq j} \frac{V_{ij}}{2} \hat{\sigma}_{ee}^{(i)} \hat{\sigma}_{ee}^{(j)}$ , where  $\Omega_M$  is the maximal Rabi coupling generated by the control lasers. The coherence  $\gamma$  as well as the phase factor  $\alpha$  for each individual initial state in  $\rho_\psi^{\text{sub}}$  will result in unique dynamics. The difference between the targeted GHZ state and any others states in  $\rho_\psi^{\text{sub}}$  is thus detectable from the differing dynamics of the excitation probabilities for one qubit,  $E_i(\rho(t)) \equiv \text{Tr}[\rho(t)|1_i\rangle \langle 1_i|]$ .

As an example, Fig. 5(a) top panel shows that the excitation dynamics of the targeted GHZ initial state (the  $\gamma = 0.5, \alpha = 0.5\pi$  state in  $\rho_\psi^{\text{sub}}$ ) differs from that of a fully mixture state, labelled as  $\rho_{\text{mix}}$ , in  $\rho_\psi^{\text{sub}}$  with  $\gamma = 0$ . The excitation difference  $D_t \equiv E_i(\rho_\psi^{\text{sub}}(t)) - E_i(\rho_{\text{GHZ}}(t))$  is a function of  $\gamma$  and  $\alpha$  for a general initial state in  $\rho_\psi^{\text{sub}}$ , where the parameter  $t$  in the brackets represents the evolution of the corresponding state from time 0 to time  $t$ . We use a notation without  $t$  to denote the time-maximal deviation within the experimental time as  $|D| = \max_t |D_t|$ . Fig. 5(a), bottom panel, depicts  $|D_t|$  for  $\rho_{\text{mix}}$ . In this example  $|D|$  occurs at about  $6 \mu\text{s}$ . This time only varies slightly by changing parameters. Fig. 5(b) depicts  $|D|$  for different  $\gamma$  and  $\alpha$ . In the small  $\gamma$  limit,  $\rho_\psi^{\text{sub}}$  is close to the fully mixed state, so that  $|D|$  is insensitive to the phase factors  $\alpha$ . For  $\gamma = 0.5$ ,  $\rho_\psi^{\text{sub}}$  consists of the GHZ states with different phase factor, and therefore  $|D|$  significantly depends on  $\alpha$ . In general, every state differs from each other in terms of  $D_t$ , and  $|D|$  is a good measure of the difference.

Thus, the detection scheme we propose is firstly measuring the excitation profile of the prepared state and then evolving the prepared state under the detection Hamiltonian to compare the dynamics of a single qubit excitation  $D_t$  with respect to that of the targeted GHZ state. The total experimental time, which is composed of the preparation time ( $t_p = 3 \mu\text{s}$ ) and the free evolution time in the second step ( $t_d = 6 \mu\text{s}$ ) plus the excitation detection time ( $t_e = 10 \mu\text{s}$  [77]), is shorter than the lifetime of the Rydberg state.

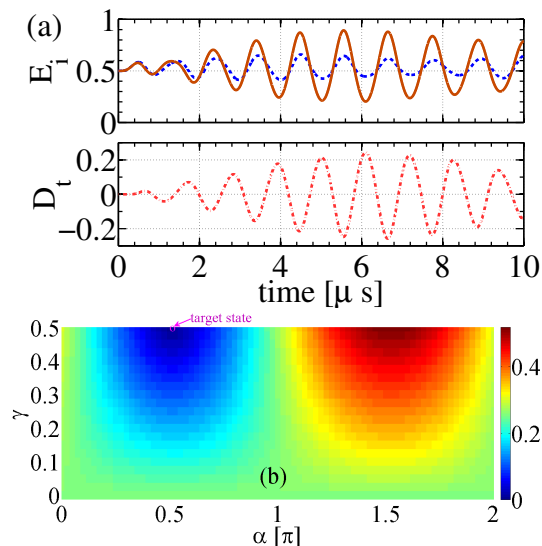


FIG. 5. GHZ state detection. (a) Evolution of the single superatom excitation under the detection Hamiltonian with different initial state: GHZ state  $(|0000\rangle + i|1111\rangle)/\sqrt{2}$  (solid brown curve), equally mixed state  $\rho_{\text{mix}} = (|0000\rangle\langle 0000| + |1111\rangle\langle 1111|)/2$  (dashed blue curve), and the deviation  $D_t = E_i(\rho_{\text{mix}}) - E_i(\rho_{\text{GHZ}}(t))$  (red dot-dash curve). Due to the symmetry of the lattice geometry all the superatoms behave the same. (b) The time-maximal deviation  $|D|$  as a function of  $\gamma$  and  $\alpha$ . The target state is highlighted with purple circle.

## V. ARBITRARY STATE PREPARATION

After showing the success of preparing two different kinds of states, either in the low energy or in the high energy region, in Rydberg atoms with the assistance of optimal control, in this section we continue to demonstrate applicability of the dCRAB method in controlling Rydberg systems through preparing arbitrary many-body superposition states in a Rydberg atomic gas, for which no other experimental approach exists. We choose the same lattice geometry and lattice defect as adopted in the GHZ state preparation scenario. Due to the symmetry of the system, all the possible states that are accessible from the  $|0000\rangle$  state must live in the space spanned by the states  $\{|S_n\rangle\}_{n=0}^4$  as  $|\psi_a\rangle = \sum_{n=0}^4 a_n |S_n\rangle$ , where  $|S_n\rangle$  is the symmetric state with  $n$  excitations, e.g.,  $|S_0\rangle = |0000\rangle$ ,  $|S_1\rangle = (|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle)/2$ , etc. The state  $|\psi_a\rangle$  is determined by the coefficients  $\{a_n\}_{n=0}^4$ . Here we assign a group of normalized random numbers  $\{0.5737, 0.5586, 0.3399, 0.3500, 0.3475\}$  to  $\{a_n\}$  as the target state. Realistic control pulses have been identified for preparing the arbitrary state  $|\psi_a\rangle$  with a high average fidelity of 0.975 over an ensemble of  $N_r = 50$  realizations, as evidenced in Fig. 6, showing the optimized control pulse [panel (a)], the tomography for the target state [panel (b)], and the tomography of the difference between the prepared state and the target state [panel (c)].

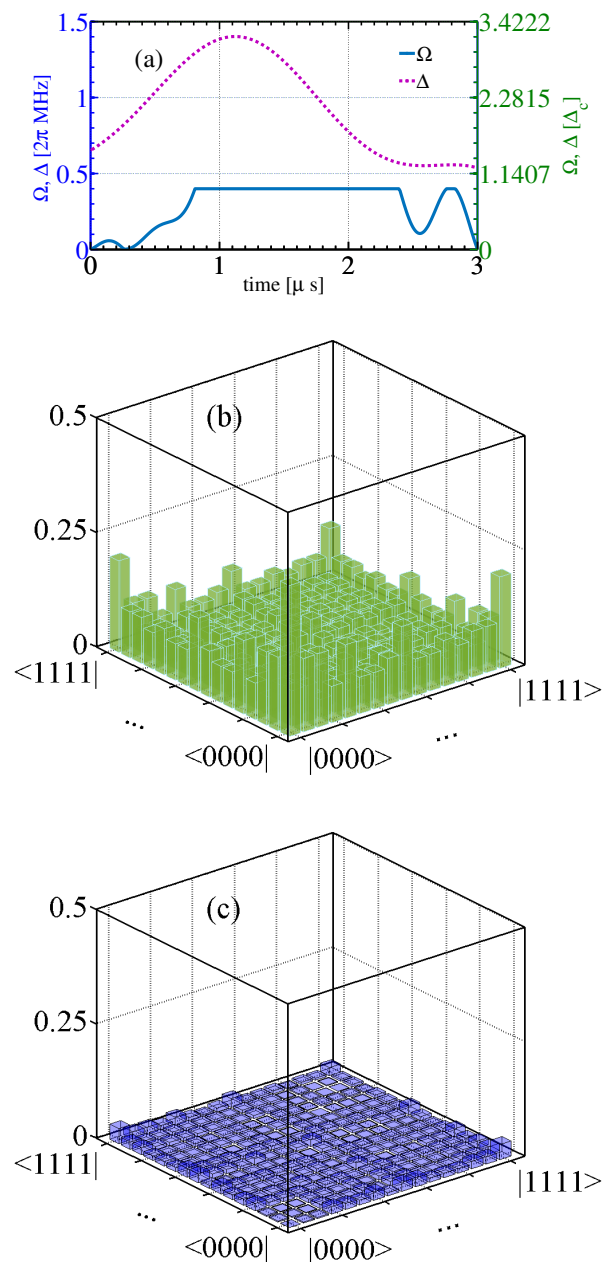


FIG. 6. Arbitrary state preparation. (a) Optimal control parameters. (b) The tomography of the target state. (c) The tomography of  $\rho(T) - |\psi_a\rangle\langle\psi_a|$ . Here  $\rho(T)$  is the average final state over 50 realizations of the system with lattice defects.

## VI. DISCUSSION AND SUMMARY

In this paper, we demonstrated an optimal control scheme to prepare a “pure” Rydberg crystal with unprecedented high fidelity. Realistic experimental constraints, such as the evolution time, the tunability range and the bandwidths of the control parameters, among others, as well as the lattice defects have been considered. Therefore, the optimized control can be readily applied in real experiments.

Furthermore, we optimized the control lasers for preparing GHZ states on the same Rydberg platform. Each logical qubit is encoded in a superatom, which is composed of a group of  $2 \times 2$  atoms, via the blockade effect. The logical qubits themselves are separated by  $8a$  along both the  $x$  and the  $y$  directions in the optical lattice to avoid the Rydberg blockade effect. This setup with superatoms improves the robustness against imperfections in the initial state filling. A two-step detection scheme for the GHZ states on this platform is also proposed here.

The applicability of the Rydberg platform combined with the dCRAB optimal control method is not limited to crystalline state and GHZ states. We report that optimal control pulses for preparing some superposition of symmetric Fock states, whose symmetry is inherited from the system Hamiltonian as translational invariance, have been calculated with single-shot fidelity larger than 0.99.

The total evolution times can be in principle further reduced without significant reduction of the fidelities until reaching the quantum speed limit times [90], which is defined as the minimum time scale for a given set of external controls to perform a particular evolution in the quantum states; however, the exploration of the quantum speed limit for preparing the given states on Rydberg system is beyond the scope of this paper.

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