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**PAPER**

**Optimal control of Rydberg lattice gases**

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**Abstract**

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 optimised 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.

**1. 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 on 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 \[46\] employed a carefully designed adiabatic pulse scheme \[22, 48–50\], 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 \[56–64\], and the design of many-body quantum dynamics \[65–67\], as well as the successful applications in experiments \[68–71\], especially those with Rydberg atoms \[63, 64, 72–74\], we adopt the ‘chopped random basis’ (CRAB) and dressed CRAB (dCRAB) optimal control method \[66, 75, 76\] for quantum state preparation in Rydberg lattice gases.

We will showcase three typical examples: (i) crystalline states of regularly spaced excitations \[46\] as a prominent and experimentally relevant example of the Rydberg blockade effect, (ii) GHZ states with maximal multipartite entanglement, relevant for quantum information processing tasks \[77–82\], and (iii) an arbitrary superposition state, for which no other preparation method is known so far, demonstrating the generality of our method.

The paper is organised as follows. In section 2 we provide a description of the Rydberg system under study, as well as an outline of the relevant experimental considerations. Section 3 demonstrates the results for the Rydberg crystalline state preparation and the obtained excitation staircase. In section 4 we show the optimised 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 section 5. Finally, section 6 summarises the paper and provides an outlook on exploring the so-called quantum speed limit of state preparation in Rydberg atoms.

2. Basic description

The system we consider is composed of a two-dimensional lattice with one atom per site, which can be realised experimentally either in an optical lattice \[46, 83\] or in an array of optical dipole traps \[2\], or even in dense disordered gases by targeted laser excitation \[84\]. Given the short time scales considered in this paper and other works in the literature \[22–25, 32–37, 46, 83, 85, 86\], only the internal electronic degrees of freedom are considered. Initially the system is prepared in the Mott insulating phase in which every atom is in its electronic ground state \[|g⟩\]. Laser light couples the atomic ground state \[|g⟩\] to a high-lying Rydberg state \[|e⟩\] with a Rabi frequency \(Ω\) and frequency detuning \(Δ\), as illustrated in figure 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 \[46, 83\] where Rubidium atoms have been excited to \(43\)S\(_1\)\(_\text{J}1\) Rydberg states via a far detuned intermediate \(5P\text{\_J2}\) state with two laser beams. This essential state picture is well justified, as near-resonant state mixing \[85, 87\] can be neglected \[22\].

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, \(V_{ij} = C_a / |\mathbf{r}_i - \mathbf{r}_j|^{6}\). For the selected 43S\(_1\)\(_\text{J}1\) state the corresponding \(C_a = 1.625 \times 10^{-60}\) J m\(^6\) \[46, 88\]. The interaction between two ground states or between one ground- and one Rydberg atom is negligible \[6, 89, 90\]. In the interaction picture, this system can be described by the Hamiltonian \[19, 46\]

\[
H(t) = \frac{\hbar}{2} \Omega(t) \sum_i \left( \hat{σ}_x^{(i)} + \hat{σ}_y^{(i)} \right) + \sum_{i<j} V_{ij} \hat{σ}_x^{(i)} \hat{σ}_x^{(j)} - \hbar \Delta(t) \sum_i \hat{σ}_z^{(i)},
\]

where the operators \(\hat{σ}_α^{(i)} = |α⟩⟨β|\) denote the atomic transition and projection operators for the \(i\)th atom at position \(\mathbf{r}_i\). We investigate the Rydberg atom excitation dynamics by integrating the Schrödinger equation governed by \(H(t)\), employing a numerical approach described in \[22, 49\].

In figure 1(c) we show the spectrum of eigen-energy levels of the system described by the Hamiltonian (1) in the classical limit \(Ω = 0\). 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-localised 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 figure 1(c). Therefore, the low-energy sector of the spectrum is composed of ordered Rydberg atom configurations which minimise the total interaction energy \[22\].

Accurate pulse shaping of the Rydberg excitation laser provides precise experimental control of both \(Ω(t)\) and \(Δ(t)\). 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 \(|gg \ldots g⟩\), with all atoms in their ground state. While the
The basic idea of this approach [22, 48, 49] has been demonstrated in recent experiments [46, 83], preparation fidelities have remained limited by lattice imperfections and unavoidable transitions between the ground state and the low-lying excited many-body eigenstates of equation (1). 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 randomised truncated Fourier basis, through iteratively updating the coefficients of the basis functions using a numerical minimisation (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 \(\Omega \leq 400\) kHz [46, 83], and imposing a truncation on the highest Fourier frequency for synthesising \(\Omega(t)\) and \(\Delta(t)\) at 8.3 MHz and 0.3 MHz, which translate into a minimum rise and fall time for \(\Omega\) and \(\Delta\) of 60 ns and 1000 ns, respectively. In this paper, we constrain the amplitude of \(\Delta\) to be within \(\pm 2\) MHz as in the experiments [46]; however, this cutoff is not a fundamental limit. We will see later that even with this limitation we can

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**Figure 1.** Rydberg atomic gas. (a) Level scheme of two \(^{87}\text{Rb}\) atoms in optical lattice sites. The atomic ground state \(|g\rangle\) is coupled, with Rabi frequency strength \(\Omega\), to an excited Rydberg state \(|e\rangle\). The laser is detuned by \(\Delta\). The two atoms are separated by a distance \(r\); the blue curve represents their mutual energy shift due to van der Waals interaction. (b) The unit-filling optical lattice is tailored into a \(3 \times N\) bar shape for the crystalline state preparation. 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 superatom. Such a system can be described as a one-dimensional chain along the \(x\) direction of \(N\) superatoms with \(\sqrt{3}\) enhanced Rabi coupling. (c) Energy spectrum of an \(N = 8\) atom chain in the classical limit \((\Omega = 0)\), plotted as a function of the detuning in units of \(V_L = C_L/L^4\), which is the interaction energy between atoms located at opposite ends of the chain, with \(L = (N-1)a\) the length of the chain. The dashed vertical line marks the phase transition point \(\Delta = 0\). Each eigenstate of the system has a well-defined total number of excitations \(N_e\), indicated by a colour code: blue \((N_e = 0)\), magenta \((N_e = 1)\), green \((N_e = 2)\), yellow \((N_e = 3)\), black \((N_e = 4\) to 7), red \((N_e = N)\). For the ground states, these excitations are regularly spaced, minimising the interaction energy and forming a crystalline state. The inset shows a zoom of the low-lying spectrum near the quantum phase transition point and the first ground state level-crossing point.
prepare high-fidelity crystalline states and GHZ states, and if we allow for larger detunings \( \Delta \) in the optimisation, the results can only improve.

Finally, in order to account for lattice defects, we consider an ensemble of \( N_r = 50 \) realisations with a lattice filling fraction of 0.9 in the optimisation. We use the average fidelity, \( F_C \equiv \langle \langle \langle \psi_C \mid \psi(r) \rangle \rangle \rangle \) and \( F_G \equiv \langle \langle \langle \psi^G \mid \psi(r) \rangle \rangle \rangle \) for crystalline state \( \mid \psi_C \rangle \) and the GHZ state \( \mid \psi^G \rangle \), respectively, as the figure of merit for the optimisation. Here the bars represent the ensemble average over \( N_r \) realisations, and \( \mid \psi(r) \rangle \) is the final state at time \( r \). This choice for the figure of merit ensures that while the obtained control parameters do not just optimise certain individual configurations but yield an optimised average dynamics with a high degree of robustness with regards to lattice defects. In this paper we neglect other sources of imperfections, such as dephasing due to instrumentation or stray fields, which were found to be of minor relevance under typical experimental conditions [46, 83].

3. Crystalline state preparation

In order to prepare a crystalline state with a given number \( N_c \) 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 figure 1(c). Such a near-adiabatic modification of the low-energy many-body states [22, 49, 91] 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 delocalised 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 \( 3 \times N \) lattice as illustrated in figure 1(b), where the lattice spacing \( a = 532 \text{ nm} \). Since the transverse extent is considerably smaller than the Rydberg blockade radius, this geometry behaves as a one-dimensional chain \( N \) superatoms and of length \( L = (N - 1) a \) with a collectively enhanced Rabi frequency \( \sqrt{3} \Omega \) [46]. As described in the previous section, our method accounts for possible lattice defects and therefore includes resulting fluctuations of the effective Rabi frequency the fluctuating number of atoms per superatom.

In figure 2(a) we show the pulse shape optimised via the dCRAB optimal control method [76] for the generation of a 3-excitation crystal in a chain of \( N = 17 \) qubits 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 figure 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
These states have the correct number of excitations and defects, the achieved positions of the actual ground state. Even though our protocol is run in an imperfectly prepared lattice with frequencies, which are now available for single-photon Rydberg excitation as recently demonstrated in [25], the total decay probability by the time evolution of the energy process, e.g. Rydberg state radiative decay, only plays a minor role on a time scale of 4 μs, as can be seen from the total decay probability \( P_d(t) = \int_0^t \Gamma N_e(t') dt' \), where \( N_e(t') = \langle \sum_i |e_i\rangle \langle e_i| \rangle \) is the total excitation number of the lifetime of the Rydberg atom.

Figure 3. Dynamics of the Rydberg crystallisation. (a) Low-lying energy spectrum of the laser-dressed system (blue dashed curve) and the energy of the instantaneous state from the optimised dynamics (red solid curve). We zoom in at the curves between 3.1 and 3.3 μs in the inset, during which the energy of the optimised dynamics goes into the excited spectrum. (b) The energy gap between the first excited state and ground state (magenta dashed curves) as well as the energy difference between the instantaneous state and the ground state (green solid curve). In the time window from 3.1 to 3.3 μs 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 \( |ψ(t)\rangle \) and the ground state \( |ψ_c(t)\rangle \). This overlap measures how close the optimised dynamics is to the adiabatic evolution. (d) Fidelity (orange curve with circle marks) and the probability of excitations with given numbers, \( P_n \), for the instantaneous state (solid curves) and the time-local ground state (dotted curves) by colour code: black, red, green, blue, magenta correspond to \( n \) from 0 to 4.

Excitation number \( n \), i.e., \( P_n = \langle \sum_i |e_i\rangle \langle e_i| \rangle \), more stringent evaluation than \( P_n \) is the state fidelity \( F_n \). Our optimal control scheme reaches a high ground state average fidelity over \( N \) imperfect realisations of \( F_n > 0.85 \) 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 employed in [46] tends to obtain states with low fidelity but relatively high \( P_n \) because of unavoidable transitions to the low-lying excited many-body Fock states. While these states have the correct number of excitations \( n \), the excitations can be slightly displaced with respect to positions of the actual ground state. Even though our protocol is run in an imperfectly prepared lattice with defects, the achieved fidelity yields a significant improvement over previous work for \( n = 3 \), 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 [22]. As shown in figure 2(c), this staircase appears as a stepwise increase of the Rydberg atom number of the many-body ground state, when increasing the system length while keeping all other parameters fixed. In order to obtain the staircase, we apply the optimised control fields for the case of \( N = 17 \) to systems of different length \( N \). As detailed in [22, 46], varying the chain length is practically equivalent to a rescaling of the applied detuning, \( \Delta \), via a change of \( V_c \) (see figure 1(c)). Hence, one can effectively target many-body ground states with different excitation numbers upon changing the chain length for fixed parameters of the excitation pulse. As shown in figure 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 [46]. For comparison, figure 2(d) shows the numerical excitation staircase obtained by using the adiabatic pulse employed in [46]).

Figure 3 illustrates the Rydberg excitation dynamics induced by our optimised laser pulse. As demonstrated by the time evolution of the energy (figure 3(a)), energy gap (figure 3(b)), the overlap between the instantaneous state and time-local ground state (figure 3(c)) as well as the excitation number distribution and the instantaneous state fidelity (figure 3(d)), the optimised system dynamics indeed remains near-adiabatic and closely follows the instantaneous many-body ground state during the first 3 μs. This suggests that adiabatic preparation methods [22, 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 optimised control pulses presented here are robust against the lattice imperfections arising from non-unity filling of atoms. Decoherence process, e.g. Rydberg state radiative decay, only plays a minor role on a time scale of 4 μs, as can be seen from the total decay probability \( P_d(t) \).
state at time $t$, and $G = 11.8 \text{ kHz}$ is the single atom radiative decay rate for the $S_{\frac{1}{2}}$ state of $^{87}\text{Rb}$ [92]. For the optimised evolution the total decay probability at the final time is only $P_{0.1}$.

Recent numerical work [50] pointed out that the preparation scheme employed in [46] would yield a rather low ground state fidelity $F \approx 0.2$ for the short pulse duration of 4 $\mu$s used in the experiment [46]. It was, hence, concluded that adiabatic crystal state preparation requires substantially longer excitations times at which dissipative processes would inevitably start to play a significant role [50]. The above results (see figures 2 and 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.

4. 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 $D_c = \sum_{ij} c_{ij}^2 / L^2$, as marked in figure 4(b), where the $N$-atom ground state, $|G\rangle \equiv |g_1, g_2, \ldots, g_N\rangle$, becomes degenerate with the fully excited state $|E\rangle \equiv |e_1, e_2, \ldots, e_N\rangle$, which allows to generate maximally entangled GHZ states, $|\psi^{(N)}\rangle = (|G\rangle + e^{i\theta}|E\rangle) / \sqrt{2}$ [86].

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 [93] as to obtain 4 qubits, each of which located at one corner of a $10 \times 10$ square lattice, see figure 4(a). 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, 94–96]. The large qubit spacing ensures a moderate interaction energy of $\hbar^{-1}c_0/(8a)^6 = 0.4125 \times 2\pi \text{ MHz}$ for the $43S_{1/2}$ Rydberg state used in [46, 83], 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. Avoiding such undesired effects once more requires very short operation times, i.e. it calls for optimised preparation pulses.

Figure 5 shows such an optimised pulse for a targeted GHZ state with $q_p = 2$ and a chosen pulse duration of 3 $\mu$s, and requiring a vanishing initial and final Rabi frequency as well as a detuning of $\Delta t = \Delta_c$ at the end of the pulse. The time evolution of the corresponding fidelity is depicted in figure 5(b) (cyan solid curve), 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 fidelity $\approx 0.95$. Such conditions and geometries can, for example, be realised with optical dipole-trap arrays as demonstrated in a number of recent experiments [2–4, 19]. As can be seen from the $P_0 + P_4$ curve in the panel (b), the optimised quantum dynamics differs significantly from the preparation protocol proposed in [86], 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 figure 5(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 μs preparation time of figure 5 is sufficiently short to ensure a total decay probability \( P_d(T) \) of less than 0.07 (see figure 5(c) the orange shaded area plotting the 10 times amplified \( P_d(t) \)). The final value \( P_f(\tau) \) provides an upper bound on infidelity caused by Rydberg state decay, assuming that any decay prevents the target state preparation. The overall preparation fidelity can thus be estimated as \( F_g \times (1 - P_d(T)) = 0.86 \). The real part and the imaginary part of the final density matrix for the prepared state (brown) and the targeted GHZ state (green) are shown in figures 5(d) and (e), respectively.

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, 83] 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 [97].

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 \( |\psi(\tau)\rangle \). 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 \( \rho_{\text{sub}}^{\text{ab}} = \frac{1}{2} \left( \frac{\gamma e^{i\theta}}{\gamma e^{-i\theta}} \right) \) with \( 0 \leq \gamma \leq 1/2 \). Clearly, the GHZ states \( |\psi_G\rangle \) are described by \( \rho_{\text{sub}}^{\text{ab}} \) 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 \( \rho_{\text{sub}}^{\text{ab}} \). 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 [98]. 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 \( H_d = \frac{\beta}{2} \Omega_{\text{tot}} \sum_i (\hat{a}_i^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{a}_i) + \sum_{i,j} \frac{\gamma_i}{\omega_{ij}} \hat{a}_i \hat{a}_j \hat{G}_{ij} \), where \( \Omega_{\text{tot}} \) 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 \( \rho_{\text{sub}}^{\text{ab}} \) will result in unique dynamics. The difference between the targeted GHZ state and any others states in \( \rho_{\text{sub}}^{\text{ab}} \) is thus detectable from the differing dynamics of the excitation probabilities for one qubit, \( E_\gamma(\rho(t)) \equiv \text{Tr} \{ \rho(t) | 11 \rangle \langle 11 | \} \).

As an example, figure 6(a) shows that the excitation dynamics of the targeted GHZ initial state (the \( \gamma = 0.5, \alpha = 0.5 \pi \) state in \( \rho_{\text{sub}}^{\text{ab}} \)) differs from that of a fully mixture state, labelled as \( \rho_{\text{max}} \), in \( \rho_{\text{sub}}^{\text{ab}} \) with \( \gamma = 0 \). The excitation difference \( D_t \equiv E_\gamma(\rho_{\text{sub}}^{\text{ab}}(t)) - E_\gamma(\rho_{\text{GHZ}}(t)) \) is a function of \( \gamma \) and \( \alpha \) for a general initial state in \( \rho_{\text{sub}}^{\text{ab}} \), 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 \( |D| = \max(|D_t|) \). Figure 6(b) depicts \( |D| \) for \( \rho_{\text{max}} \). In this example \( |D| \) occurs at about 6 μs. This time only varies slightly by changing parameters. Figure 6(c) depicts \( |D \) for different \( \gamma \) and \( \alpha \). In the small \( \gamma \) limit, \( \rho_{\text{sub}}^{\text{ab}} \) is close to the fully mixed state, so that \( |D| \) is insensitive to the phase factors \( \alpha \). For \( \gamma = 0.5, \rho_{\text{sub}}^{\text{ab}} \) 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 \( (t_p = 3 \mu s) \) and the free-evolution time in the second step \( (t_e = 6 \mu s) \) plus the excitation detection time \( (t_d = 10 \mu s [83]) \), is shorter than the lifetime of the Rydberg state.

5. Arbitrary state preparation

Let us finally demonstrate the general applicability of the method by studying the preparation of arbitrary many-body states in a Rydberg lattice. As a specific example we choose the same lattice geometry as in section 4 and consider symmetric target states, \( |\psi\rangle = \sum_i a_i |s_i\rangle \), spanned by the number states \( |s_0\rangle = |0000\rangle \), \( |s_\uparrow\rangle = (|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle)/2 \), etc. Again we implement realistic experimental constraints for the excitation pulse and account for random lattice defects by performing an ensemble average over 50 random spatial configurations.

In figure 7(a) we show the optimised excitation pulse for preparing the state \( |\psi\rangle \) with randomly generated coefficients, \( a_0 = 0.5737, a_1 = 0.5386, a_2 = 0.3399, a_3 = 0.3500 \) and \( a_4 = 0.3475 \). Even for a short
preparation time of 3 μs the optimised pulse allows to generate the target state with a high fidelity of 0.975. This is illustrated in figure 7(b) where we show the difference between the target state and the generated state. Its elements are very small throughout demonstrating the high quality of the optimised state preparation approach.

6. Discussion and summary

In this work, we have investigated the applicability of optimal control approaches for the dynamical preparation of many-body states in a lattice of interacting Rydberg atoms. We have demonstrated that this opens up the fidelity preparation of ordered ground states, highly entangled GHZ states and even arbitrary, randomly chosen, many-body states under realistic conditions and typical experimental constraints on excitation pulse shaping. In particular, for the latter optimal control techniques as demonstrated in this work presently provide the only suitable approach to generate complex many-body states in an efficient and experimentally viable fashion. We have placed particular focus on limitations and imperfections, such as lattice defects, that are practically unavoidable in experiments. Our optimised control pulses are robust against lattice defects, in the sense that they yield high preparation fidelities for nearly every randomly sampled spatial configuration and a high average fidelity with a small statistical spread. For example, comparing the average fidelities from two sets of 50 random samples we found a difference of less than 10^{-3} for all three studied target states.

Table 1 summarises the overall performance of the dCRAB optimal control method for the three example states. As one can see the major limitation on achievable fidelities in all three cases stems from the finite fraction of lattice defects and spontaneous decay of the Rydberg state. While we have considered here a filling fraction of 0.9 [46], recent experiments have already reached considerably higher values in optical lattices [25, 99] and optical dipole-trap arrays [3, 4]. Equally important, spontaneous Rydberg state decay ultimately limits achievable preparation fidelities, which is why we have chosen relatively short pulse durations of a few μs (see table 1).
Within our optimisation approach, it should be possible to further reduce the total evolution time without a significant degradation of the preparation fidelity until reaching the quantum speed limit. Since the preparation time eventually determines the extent of undesired decoherence effects, the detailed exploration of the quantum speed limit in Rydberg lattices presents both a fundamentally interesting and practically important problem for future studies. In view of the recent advances in optically controlling the many-body dynamics of Rydberg atom lattices, the control techniques demonstrated in this work will enhance the capabilities of such systems for quantum simulations as well as the collective preparation of complex nonclassical many-body states for quantum information applications. We hope that the first theoretical steps in this direction, as presented in this article, will initiate further experimental and theoretical work to tap the full potential of optimal control techniques for Rydberg atom many-body physics.
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