Arrays of single atoms trapped in optical tweezers and excited to Rydberg states are a promising platform for quantum simulation [1–5] and quantum information processing [6]. They combine a hyperfine qubit with demonstrated individual control and one-qubit gates with high fidelities [7–9], the possibility to scale the system to large numbers of qubits [10–12] and strong interactions. Coherent ground-Rydberg Rabi oscillations have been observed in dilute gases [13, 14], in single atoms [15–18] and in blockaded ensemble “superatoms” [19–21]. Long coherence times of ground-Rydberg Rabi oscillations are a crucial element in the context of both quantum simulation, to accurately emulate interacting systems and study their ground-state or dynamical properties [2–4, 22–24], and quantum information processing, for the implementation of two-qubit gates. Recent experimental efforts have shown an improvement in the fidelities of two-qubit gates [25, 26], but they still remain below their theoretically predicted intrinsic fidelities [27, 28], as compared to other experimental platforms such as trapped ions [29, 30] or superconducting qubits [31–33]. Part of this is due to imperfections in the coherent optical excitation of single atoms to Rydberg states.

In all such experiments reported so far, one observes that the optically driven Rabi oscillations between the ground state \( |g\rangle \) and the targeted Rydberg state \( |r\rangle \) are damped and have a finite contrast. Figure 1 gives a typical example; similar behaviors are observed in other setups [3, 18, 21, 34, 35]. Typical 1/e damping times, for a 2 MHz Rabi frequency, are about 5 \( \mu \)s, much lower than the lifetime of Rydberg states, in the \( \sim 200 \mu \)s range. This limits for instance the fidelity of preparation of \( |r\rangle \) by a \( \pi \)-pulse to about 95%. The purpose of the present study is to understand quantitatively the origins of these limitations.

As we shall see below, they arise from the combination of several small effects due to technical imperfections in the experiment. As trying to decrease one type of imperfection may actually enhance another one, it is desirable to have a detailed understanding of all the effects at play in order to reach for the best experimental trade-off. To do so we model these imperfections as simply as possible, and compare the predictions of our models with the observed behavior, sometimes by deliberately increasing the magnitude of the deleterious effects.

This article is organized as follows: after briefly recalling the characteristics of our setup, we review and quantify (i) the finite efficiencies of state preparation and detection, that give a finite contrast for the Rabi flopping, but without any damping, and (ii) the effects giving rise to damping or dephasing, among which the most significant ones are the Doppler effect, the spontaneous emission \( \text{via} \) the intermediate state used for the two-photon excitation, and the laser phase noise. Then, combining all the effects in a global simulation, we compare with experimental results and discuss possible routes towards an improvement of the fidelities.

I. EXPERIMENTAL SETUP

The geometry of our experimental setup [2] is shown in Fig. 2(a). A Rydberg excitation sequence is as follows. We first check for the presence of a single \(^{87}\text{Rb}\) atom in the 1 mK-deep tweezers by shining the molasses beams during 50 ms and collecting the fluorescence photons on an EMCCD camera. The atom is then cooled from a temperature of \( 60 \mu \text{K} \) after imaging to about \( T = 30 \mu \text{K} \) by first increasing the detuning of the molasses beam and then by adiabatic lowering of the trap depth [36]. An external magnetic field along \( z \) of typically 7 G is then switched on to define the quantization axis, and, after 50 ms, we optically pump the atom into the...
II. STATE PREPARATION AND DETECTION ERRORS

Even if the excitation process of an atom in |g⟩ to the Rydberg state |r⟩ were perfect, the measured recapture probability would not show perfectly contrasted oscillations due to state preparation and measurement errors (‘SPAM’ errors). We identify three different components: (a) the finite efficiency of the optical pumping leading to a preparation error with probability η, (b) the “false positive” errors in the Rydberg detection, as we have a probability ε = P(r|g) to incorrectly infer that a ground-state atom was in |r⟩ because it was lost, e.g. due to background-gas collisions, and (c) the “false negative” errors, with a probability ε’ = P(g|r) to recapture a Rydberg atom which has quickly decayed back to the ground-state.

We denote by Pg and Pr the actual population of the states |g⟩ and |r⟩ due to the evolution of the system under the excitation laser, possibly in the presence of the damping and dephasing mechanisms to be discussed in Sec. III. Due to the nonzero values of (η, ε, ε’), the measured probabilities of recapture Pg and of loss Pr are slightly altered and become:

\[ P_g = \eta (1 - \varepsilon) + (1 - \eta)(1 - \varepsilon) \left( \tilde{P}_g + \varepsilon' \tilde{P}_r \right), \]
\[ P_r = \eta \varepsilon + (1 - \eta) \left( \varepsilon \tilde{P}_g + (1 - \varepsilon' + \varepsilon \varepsilon') \tilde{P}_r \right). \]

It implies that, even if the “real” population \( \tilde{P}_r \) undergoes a perfect Rabi oscillation \( \tilde{P}_r(t) = \sin^2(\Omega T/2) \), the measured one \( P_r(t) \) has a finite contrast. Figure 3 illustrates the effect to lowest order in (ε, ε’, η). In principle, one can invert the above equations [38], e.g. using a maximum likelihood procedure, to correct the measured populations for these errors and recover the “real” populations, even for many qubits [3]. In our publications we however include these SPAM errors on the theoretically calculated populations when comparing with data [2, 39]. In the following, we investigate in detail the causes of those ‘SPAM’ errors.

a. Efficiency of optical pumping. The optical pumping into |g⟩ is not entirely perfect, and we denote by η the probability that after optical pumping, the atom is not in |g⟩ but in another Zeeman or hyperfine state of 5S1/2. Measurements using microwave transitions between the two hyperfine levels of 5S1/2 allow us to estimate an upper-bound on the preparation error η < 0.005.

b. Detection errors: false positives. The detection of the final state of the atom relies on its recapture, which ideally always occurs if the atom is in |g⟩, and never occurs if it is in |r⟩. However, there is a finite probability ε to lose a ground-state atom during the sequence. A first source of errors are collisions of the single atom with the background gas, which gives a vacuum-limited lifetime of 20 s for an atom in the 1 mK deep tweezers without any cooling light. Integrated over the ~ 50 ms required to perform the experiment (limited by eddy currents when switching off the external B-field), it amounts...
to an error rate of 0.3%. During the fluorescence imaging, when the molasses beam is turned on, the single atom lifetime is reduced to 8 s while the atom temperature does not increase. This could be due to the trapped atom dynamics under illumination with cooling light [40] or to residual loading from background Rb vapor. The atom can thus leave the trap during the 50 ns fluorescence images and we estimate that this second cause of detection errors amount to 0.6%. A third reason for losing the atom comes from its displacement, due to its finite temperature $T$, when the optical tweezers is switched off during the experimental time $\tau$, as explained in Appendix A. We calculate that the probability for this event remains below 1% for $T = 30 \mu K$ and $\tau < 6 \mu s$, such that by adding all three contributions we predict a false positive rate $\varepsilon < 2\%$. When measuring it by repeating the experimental sequence described in Sec. I with the traps switched off during a time $\tau \approx 1 - 6 \mu s$ but without shining the excitation beam, we indeed obtain a typical loss rate $\varepsilon \approx 1 - 2\%$, in good agreement with the above estimate.

c. Detection errors: false negatives. Conversely, an atom that has been excited to $|r\rangle$ has a small but nonzero probability to be recaptured as it can decay back to the trapped ground state before having been expelled from the trapping region. An atom in $|r\rangle$ is repelled by the optical tweezers due to the ponderomotive force (see Appendix A). The effect is well captured by a measured characteristic time $t_{recap} = 10 \mu s$ during which a Rydberg atom stays in the trapping region. The probability of false negative $\varepsilon' = P(g|r)$ is then directly linked to the rate $\Gamma_R$ at which a Rydberg state decays to the ground-state (via low-lying excited states), which scales with the principal quantum number as $n^{-3}$. For $n > 50$, $t_{recap}$ is much shorter than the inverse decay rate $\Gamma_R^{-1} > 100 \mu s$ and we can approximate $\varepsilon'$ by $\Gamma_R/t_{recap}$ (Fig. 4, solid black curve). For lower $n$, the approximation is not valid anymore and $\varepsilon'$ is given by Eq. (A1) (solid red curve). We measure the detection error by (i) exciting the atom to $|r\rangle$ with probability $P_r$, (ii) pushing out, with unit efficiency, atoms still in $|g\rangle$ [41], and (iii) observing the presence or absence of the atom, which effectively measures $\varepsilon' P_r$. Together with the measurement of $P_r$ and Eq. (2), we extract the real Rydberg fraction $P_r$ and the false detection error rate $\varepsilon'$. The results obtained for Rydberg states ranging from $n = 20$ to 90 (disks) show the expected $n^{-3}$ scaling and are in quantitative agreement with our model. In our experiments, we use $n > 50$ Rydberg state and the false negative rate is limited to $\varepsilon' < 0.05$. This error becomes more severe with tweezers schemes also trapping Rydberg states as proposed in [42]. To improve this detection method, one could consider, e.g. ionizing the Rydberg atoms by applying a strong electric field.

III. DAMPING OF THE RABI OSCILLATIONS

We now turn to effects that lead to a decreasing amplitude of the Rabi oscillation when the excitation time $\tau$ increases.

A. Doppler effect

The first contribution to damping is the Doppler effect. In our setup (Fig. 2(a)), the two excitation lasers with wavevectors $k_t$ and $k_b$ are orthogonal to each other, resulting in an effective wavevector of magnitude $k_{eff} \simeq 1.5 \times 10^7 \text{ m}^{-1}$. A temperature $T = 30 \mu K$ corresponds to a one-dimensional r.m.s. velocity spread $\Delta v = \sqrt{k_B T/m} \approx 50 \text{ mm/s}$. This means that for each realization of the experiment, the detuning of the excitation laser seen by the atom is a random variable with a centered Gaussian probability distribution of standard deviation $k_{eff} \Delta v \sim 2\pi \times 120 \text{ kHz}$. Figure 5 shows the calculated influence of the Doppler effect for various Rabi frequencies $\Omega/(2\pi)$. One can see that below 1 MHz, the Doppler effect is a very significant source of dephasing, while from 1 MHz up the effect is hardly noticeable.

If we exclude more technically demanding ways to substantially decrease the Doppler effect, e.g. by using three-photon...
excitation [43] or reducing the temperature by Raman cooling [44, 45], the above results seem to indicate that one should use high Rabi frequencies. However this is not the case, because a competing effect arises, namely spontaneous emission via the intermediate $5P_{1/2}$ state.

### B. Spontaneous emission from intermediate state

Although the intermediate state detuning $\Delta$ is large compared to $\Omega_{r,b}$, there is still a small probability for the atom to be in the intermediate state $|p\rangle$, which has a natural linewidth $\Gamma \simeq 2\pi \times 6$ MHz. From $|p\rangle$, the atom decays back to $|g\rangle$ with a probability $1/3$, and to the other sublevels of $5S_{1/2}$ with a probability $2/3$.

To take into account this spontaneous emission in the simplest way, we use a 4-level model for the atoms [17], with the states $|g\rangle$, $|r\rangle$, $|p\rangle$ and an extra state $|g'\rangle$ which accounts for all the ground-state sublevels, other than $|g\rangle$, to which the atom can decay from $|p\rangle$ (see Figure 2b). We solve the optical Bloch equations (OBEs) for the density matrix $\rho$:

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}[H, \rho] + \mathcal{L}[\rho]$$

where the Hamiltonian reads, in the rotating wave approximation,

$$H = \frac{\Omega_r}{2} \left( \langle g | p \rangle \langle p | g \rangle + \frac{\Omega_b}{2} \left( \langle r | p \rangle \langle p | r \rangle + \langle p | r \rangle \langle r | p \rangle \right) - \Delta \langle p | p \rangle - \delta |r\rangle \langle r |. \right.$$

(4)

Here $\delta$ is the (small) detuning from the two-photon resonance condition. The dissipator has the Lindblad form:

$$\mathcal{L}[\rho] = \sum_{i=g,g',r} \tau_i^p \left( \frac{\Gamma_i}{2} (2i\rangle \langle i | \rho | p \rangle | p \rangle \langle i | - | p \rangle \langle p | \rho - \rho | p \rangle \langle p |) \right),$$

(6)

with $\Gamma_g = \Gamma/3$ and $\Gamma_{g'} = 2\Gamma/3$. Here, decay of $|r\rangle$ is neglected (see Sec. III D). The recapture probability is then $1 - \rho_{rr}$.

Figure 6(a,b) shows the results of such simulations for the values of $\Omega_b$ and $\Delta$ that we generally use. The two-photon detuning $\delta$ was adjusted to compensate for the light-shifts $(\Omega_r^2 - \Omega_b^2)/(4\Delta)$. When increasing $\Omega_r$ we observe a stronger and stronger damping, which also shows a characteristic asymmetry: the successive maxima of $P_r$ become significantly smaller, while the minima remain quite close to zero. This is simple to understand: spontaneous emission via $|p\rangle$ slowly optically pumps the atoms into the dark state $|g'\rangle$, and these atoms will be detected as ground-state atoms, even though, not being any more in $|g\rangle$, they have no possibility of being excited to $|r\rangle$.

In Fig. 6(c,d) we compare the prediction of the simulation to experimental data where we reduced $\Delta$ to enhance on purpose the effects of spontaneous emission. We get a good agreement (without adjustable parameters), giving confidence in the simple model we use. We note that the problem of spontaneous emission from an intermediate state is avoided when using a direct single-photon excitation scheme [18] or minimized when choosing a higher intermediate state with smaller natural linewidth (for instance, when using an “inverted” two photon scheme as in [3], the linewidth of the intermediate $6P_{1/2}$ state is only 1.3 MHz).

### C. Laser phase noise

Another important effect giving rise to damping of the oscillations is the fact that the excitation lasers have finite phase noise. We use two extended-cavity diode lasers (ECDLs), one at 795 nm, and one at 950 nm which is amplified in a tapered amplifier and frequency-doubled in a resonant cavity. Both ECDLs are locked using the Pound-Drever-Hall (PDH) technique on a high-finesse ultra-stable ULE cavity ($f \sim 20,000$ for both wavelengths). Their phases $\phi_i(t)$ ($i = 795, 950$) are random processes with a power spectral density $S_{\phi_i}(f)$, where $f$ denotes the Fourier frequency. Measuring $S_{\phi_i}(f)$ directly is not an easy task, but we obtain a reasonable estimate of $S_{\phi_i}(f)$ for Fourier frequencies $f$ above acoustic frequencies, where the cavity noise is negligible, by analyzing the in-loop PDH error signal with an RF spectrum analyzer: the noise spectral density of the PDH error signal voltage allows to retrieve $S_{\phi_i}(f)$, knowing the slope of the PDH error signal at the lock point and taking into account the storage time of light in the cavity which causes a roll-off of the cavity response to frequency fluctuations (see e.g. [46], page 17).

Figure 7(a) shows the spectral density of frequency noise $S_{\phi_i}(f)$, which is related to the phase noise spectral density by $S_{\phi_i}(f) = f^2 S_{\phi_i}(f)$ [47]. The solid lines represent the typical frequency noise measured when operating the experiment. We observe a broad maximum of noise around 1 MHz, due to the limited feedback loop bandwidth, which implies that...
The influence of laser phase noise. (a): Estimated spectral density $S_\nu(f)$ of the frequency noise of the 795 nm (red) and 950 nm laser (blue). Solid lines: usual noise, dashed line: enhanced noise (see text). (b): Simulated Rabi oscillation in the presence of usual phase noise. Many Rabi oscillations (thin lines), each for a given realization of the random processes $\phi_i(t)$, are averaged (thick black line). (c): With intentional extra noise added in the 950 nm laser the damping is increased, and the simulation compares well with the experimentally observed Rabi oscillation on $n = 54$ (red circles).

Several other effects can in principle contribute to damping and dephasing of the Rabi oscillations. First, the Rydberg states have a finite lifetime due to spontaneous emission leading to decay to low-lying excited states and to black-body radiation transferring the atom to close-by Rydberg states [51]. The latter has been shown to be detrimental to Rydberg-dressing experiments with many particles [52, 53]. We have solved the OBEs with and without including the finite lifetime of Rydberg states $n > 50$ and observed no significant differences on the timescale of a few microseconds for the single-atom Rabi oscillation. Thus, so far, this finite lifetime is not a limitation in our setup.

If the excitation beams are not perfectly centered on the trap position, the atom sits on a spatial gradient of Rabi frequency and light-shift, and thus its random thermal motion from shot to shot gives rise to dephasing. We have checked that for our experimental parameters, this effect should be negligible unless the excitation beams are strongly misaligned. Another dephasing mechanism is the shot-to-shot variation in the pulse areas of the excitation beams. We have estimated the relative fluctuations of the intensity of the pulses to be below 0.2% rms, which does not lead to any measurable dephasing over our experimental timescales.

Finally, stray transverse electric fields leading to mixing between different Zeeman sublevels of the targeted Rydberg state could lead to a degradation of the Rabi oscillation, as $|g\rangle$ would be coupled to several Rydberg states with different coupling strengths. However, using eight independent electrodes under vacuum, we zero out the electric field to better than $|E| < 5$ mV/cm by performing Stark spectroscopy on high-$n$ Rydberg states (typically $n \sim 100$). For such low values of $E$, the expected effect of stray fields is negligible.

### IV. COMBINING ALL EFFECTS; PROSPECTS FOR IMPROVEMENT

Having developed a quantitative modeling of each of the experimentally relevant imperfections listed above, we can...
now include them all in a global simulation. All parameters (Rabi frequencies of the red and blue lasers, detuning Δ, SPAM errors (η, ε, ε′), atomic temperature T, spectral density of the phase noise of lasers...) are given their independently measured values. We draw fluctuating parameters according to their respective distributions, integrate the OBEs with these parameters, and then average over typically 600 realizations. Figure 8(a) shows a comparison between an experimental Rabi oscillation (for Ω/(2π) = 4.8 MHz, disks) and a parameter-free simulation (solid line) including all effects detailed in this work. The fair agreement between data and simulation allows us to explore, using our numerical simulation, how varying experimental parameters affects the coherence of the Rabi oscillation.

As an example, we show in Fig. 8(b) how the different effects depend on the Rabi frequency Ω. The simulations are performed for a fixed Rabi frequency of the blue laser Ωb/(2π) = 35 MHz (typical for n ~ 60) and a varying red laser Rabi frequency Ωr. To characterize the damping of the Rabi oscillation, we extract from the simulations the oscillation amplitude during the fifth half-period [gray shaded in Fig. 8(a)]. When including all effects in the simulation (red solid line), we observe that the damping is minimized for Ω/(2π) ≈ 2 MHz. For Ω/(2π) < 0.7 MHz, the Doppler effect (dash-dotted line) is the dominant source of damping. The phase noise influence (dotted line) peaks at Ω/(2π) = 1 MHz as predicted from its broad maximum seen in Fig. 7(a). The detrimental effect of spontaneous emission (dashed line) is minimized when Ωr = Ωb, giving Ω/(2π) = 0.8 MHz for our current parameters.

One could possibly improve the coherence by increasing the power or decreasing the size of the blue beam, thus increasing Ωblue, which would allow, for a fixed Ω, to increase Δ and thus reduce spontaneous emission. However, too small a beam waist will increase sensitivity to beam pointing instability, and, more importantly, will limit the size of the tweezers arrays that can be excited homogeneously [54], so ideally higher powers for the 475 nm laser would be needed. Another solution is to use the inverted excitation scheme, with intermediate state |6P3/2⟩, which has the combined advantage of having a longer lifetime (~ 120 ns) and better coupling to Rydberg states (at 1013 nm). Using this scheme, the Harvard group obtained promising coherence times [3, 55].

So far we have discussed only experimental situations in which the coherent laser drive is continuously on, which is relevant e.g. for the quantum simulation of Ising models [2, 3]. However, for implementing quantum gates [6], or for the quantum simulation of XY quantum magnets [39], one is interested in exciting or de-exciting selected atoms quickly and efficiently. This can be accomplished with π-pulses, in which case we are back to the problem of minimizing the decoherence of Rabi oscillations, but other schemes can be used, such as STIRAP [13, 37, 56, 57], which has the advantage of being more forgiving in terms of fine tuning of parameters. We believe that the modeling of experimental imperfections developed in this work will be useful for finding realistic optimum parameters in those scenarios.

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Appendix A: A simple model for ε′

In this appendix, we derive, using a simple model, the value of the probability ε′ for false negatives. Let us assume that, at t = 0, just at the end of the excitation sequence, the atom is in |r⟩. We then switch on the tweezers again, and after a delay of about 10 ms (due to the time it takes to open mechanical
shutters, for instance), the molasses light, in order to excite fluorescence of the atom if it is in $|g\rangle$. For the atom to emit fluorescence at the end, and thus give a false negative, it needs (i) to decay to $|g\rangle$ at some time $t$, and (ii) to be recaptured in the tweezers after having spent a time $t$ in $|r\rangle$ in the presence of the tweezers. This means that $\varepsilon'$ is given by

$$\varepsilon' = \int_0^{\infty} p_{\text{recap}}(t) \dot{\rho}_g(t) \, dt. \tag{A1}$$

In this expression, the quantity $p_{\text{recap}}(t)$ is the probability for an atom in $|g\rangle$ to be recaptured by the (attractive) trapping potential $U(r)$ of the tweezers after having experienced, for a duration $t$, the anti-trapping potential $-\alpha U(r)$. $\dot{\rho}_g(t)$ is the time derivative of the population of $|g\rangle$ when the atom is initially in $|r\rangle$, and, finally, the upper limit of the integral can safely be replaced by $+\infty$ because the time it takes to switch on the molasses light is long compared to the timescales over which the integrand is non zero (tens of $\mu$s). The ratio $\alpha$ of the anti-trapping of $|r\rangle$ and trapping potentials of $|g\rangle$ depends on the trap laser frequency $\nu$. Assuming that the potential experienced by the Rydberg atom is essentially the ponderomotive potential exerted by the tweezers on the nearby-free valence electron, we obtain $\alpha = (\nu + \nu_0)(\nu - \nu_0) / \nu^2 \approx 0.17$ (the trap laser at 852 nm corresponds to $\nu = 352$ THz, and $\nu_0 \approx 382$ THz is the average frequency of the D lines of Rb).

To evaluate (A1), we first focus on $p_{\text{recap}}(t)$. We show in Fig. 9 the effect of the anti-trapping potential on a Rydberg state $|r\rangle$ compared to a free flying atom. The theoretical curves are obtained with a Monte-Carlo simulation of the classical dynamics of a particle at temperature $T = 20 \mu$K either in a repulsive potential $-\alpha U(r)$ (solid line), either in free flight (dashed line). In a first experiment (squares), we excite an atom to $|r\rangle$ with a $\pi$-pulse, switch on the trap for a variable time $t$ and de-excite it back with a second $\pi$-pulse. The reduced contrast of the experimental data with respect to the simulation is due to the finite efficiency of Rydberg (de-)excitation. In a second experiment (circles), we simply measure the recapture probability of an atom in free flight by switching off the trap during a time $t$. Our models are in excellent agreement with the experimental data. We observe that the release and recapture measurement [36] of a Rydberg atom $|r\rangle$ is strongly affected by the slight anti-trapping and drops quickly to zero after $\sim 10 \mu$s. This anti-trapping thus plays an important role in our detection scheme, where we need the Rydberg atom to leave the trapping region as fast as possible before it decays back to the ground state.

Concerning $\dot{\rho}_g(t)$, we can write it as $\Gamma_R \exp(-t\Gamma_R)$, where $\Gamma_R$ is the rate at which a Rydberg state decays back to the ground state [51]. At finite temperature black-body radiation does increase the depopulation rate of $|r\rangle$, but by transferring population to neighboring long-lived Rydberg states, and thus it hardly affects the rate at which $|g\rangle$ gets populated.

For values of $n > 50$, the zero-temperature lifetimes $1/\Gamma_R \propto n^3$ of $|r\rangle$ are in excess of 100 $\mu$s, while the variations of $p_{\text{recap}}(t)$ occur on just a few microseconds. One can thus approximate (A1) by $\varepsilon' = \Gamma_R t_{\text{recap}}$, where $t_{\text{recap}} = \int_0^{\infty} p_{\text{recap}}(t) \, dt \approx 10 \mu$s is extracted from Fig. 9 and varies only logarithmically with the atomic temperature.

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