

Light-assisted collisions in tweezer-trapped lanthanides

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We present a quantitative investigation of one- and two-body light-mediated processes that occur to few erbium atoms in an optical tweezer, when exposed to near-resonant light. In order to study the intertwined effects of recoil heating, cooling, and light-assisted collisions, we develop a first-principles Monte Carlo algorithm that solves the coupled dynamics of both the internal and external degrees of freedom of the atoms. After validating our theoretical model against experimental data, we use the predictive power of our code to guide our experiment and, in particular, we explore the performance of different transitions of erbium for light-assisted collisions in terms of their efficiency and fidelity for single-atom preparation.

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I. INTRODUCTION

Arrays of individual laser-cooled neutral atoms in optical tweezers are a promising and fast-developing platform for an ever increasing number of applications in quantum science and technology [1–3]. Achieving the single-atom regime with high loading probability and fidelity is a key step toward successfully delivering scalable quantum architectures. In recent years, atom-array experiments have made remarkable advances in this direction, primarily using alkali [4–6] and alkaline-earth species [7–10]. More recently, a new frontier is emerging with lanthanides [11,12], which offer several intriguing advantages in state control and manipulation thanks to their complex many-electron valence structure and rich atomic spectra [13]. For instance, lanthanide spectra exhibit a diverse range of optical transitions, spanning from strong ultraviolet transitions with linewidths on the order of tens of megahertz to narrow intercombination lines of few to few hundred kilohertz [14], and clock-type transitions [15,16].

The linewidth of a given transition fundamentally determines the rate at which the internal degrees of freedom evolve, playing a pivotal role in atom-light interactions. This characteristic is crucial for understanding laser cooling, light-assisted collisions (LACs), and fluorescence imaging in atom-array experiments. For instance, in the case of alkali, fast pairwise collisions are assisted by light that is near-resonant to the megahertz-strong D-line, which is also responsible

for Doppler cooling [17,18]. During tweezer loading from a magneto-optical trap (MOT), the system is in the so-called collisional blockade regime [17,19]. Here, the loading rate balances the pair-ejection rate induced by the LACs, directly leading to single-atom preparation with efficiencies ranging from 50% to >90% for red- to blue-detuned D-line light [19–23].

In lanthanides, the situation is different. The main resonant transition used for MOT is a narrow intercombination line. This line—with no equivalent in alkali atoms—has proven to be particularly powerful since it allows for rapid and deep Doppler cooling, accompanied by simultaneous spin polarization [24], a simplified five-beam MOT [25], and nondestructive continuous imaging [11,12] that is crucial for tweezer rearrangement. The remaining question is whether this same transition can also enable fast single-atom preparation with low fraction of two-atom population in optical tweezers via LACs. Experiments have shown that this transition does not naturally reach the collisional blockade regime [20] and instead requires a dedicated LACs pulse stage [11,12,26–28]. In this context, however, a precise theoretical framework describing atom-light interactions in lanthanides is still lacking. In these systems, the timescales of atomic motion and internal-state dynamics are comparable and, unlike in alkali atoms, cannot be treated separately—posing a significant challenge for accurate modeling.

In this work, we study the dynamics of a few erbium atoms confined in optical tweezers and interacting with near-resonant intercombination light, leading to two key phenomena: two-body LACs and single-atom absorption-emission cycles accompanied by recoil heating. To capture this complex behavior, we develop a Monte Carlo (MC) algorithm that demonstrates predictive accuracy without relying on fitting parameters, as benchmarked against experimental results. Using this framework, we explore a broad parameter space and identify conditions where intercombination

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light enables in-trap Doppler cooling, effectively counteracting heating and enhancing single-atom survival. Furthermore, our simulations disentangle the contributions of recoil heating and LACs, revealing new optimal strategies for high-fidelity single-atom loading in optical tweezers. Our findings go beyond erbium by addressing generic mechanisms that emerge in optical tweezers operated with multielectron atoms. Many lanthanide species currently explored for quantum science—such as Yb, Dy, and Ho—share key structural features, including rich atomic spectrum. While quantitative differences remain species dependent, the qualitative behavior identified here is expected to persist across this broader class of atoms, making our results directly relevant to ongoing and future tweezer-based experiments.

II. METHODS

MC methods have proven to be powerful for modeling tweezer-trapped neutral atom systems, enabling extraction of few-body temperatures [29], two-body scattering and LACs rates in alkalis [30,31], and cooling dynamics including Doppler and sub-Doppler effects [32]. However, existing models often treat one- and two-body processes separately. Here, we present MC simulations that simultaneously capture the internal and external dynamics of up to three atoms in a tweezer trap under continuous illumination by one or two near-resonant beams with arbitrary propagation directions, enabling exploration of a broad range of experimental conditions. The key steps of the MC algorithm are summarized here, whereas a detailed description is provided in the Supplemental Material [28].

We consider erbium atoms trapped in an optical tweezer, operating at a magic wavelength [12]. The atoms are illuminated by light near-resonant with the intercombination transition at $\lambda_L = 583$ nm (yellow light), with linewidth $\Gamma_L/(2\pi) = 186$ kHz. Either a single horizontal or two yellow beams ($q = \{h, v\}$) are used, propagating along horizontal and vertical axes with intensities I_q . The yellow light drives both one- and two-body processes; see Figs. 1(a) and 1(b), respectively. The one-body process [panel (a)] involves single-atom scattering at rate $R_{\text{scatt}}(s_{0,q}, \Delta_{i,q}) = (s_{0,q} \Gamma_L/2)/(1 + s_{0,q} + (2\Delta_{i,q}/\Gamma_L)^2)$, where $s_{0,q} = I_q/I_{\text{sat}}$ is the saturation parameter and $\Delta_{i,q} = \Delta_q - \mathbf{k}_q \cdot \mathbf{v}_i$ is the Doppler-shifted detuning seen by atom i [33]. The two-body process [panel (b)] involves the mixing between $|g\rangle : [\text{Xe}] 4f^{12}(^3H_6)6s^2(^1S_0)$ and $|e\rangle : [\text{Xe}] 4f^{12}(^3H_6)6s6p(^3P_1)(6, 1)_7^o$, which induces a dipole-dipole interaction (DDI), driving LACs and possibly resulting in pair ejections [34]. Initially, the atom's positions $\mathbf{r}_i$ and velocities $\mathbf{v}_i$ are drawn from a thermal distribution and then evolve in time according to the following equation of motion:

$$m\ddot{\mathbf{r}}_i = -\nabla_i[V_{\text{tw}}(\mathbf{r}_i) + V_{\text{int}}(r)] + m\mathbf{g}, \quad (1)$$

where $V_{\text{tw}}(\mathbf{r}_i)$ is the tweezer trapping potential (following a Gaussian profile [28]), and $V_{\text{int}}(r) = C_3/r^3$, with $r \equiv |\mathbf{r}_i - \mathbf{r}_j|$, is the DDI between the excited atom (i) and the ground-state atom closest to it (j). Here, $C_3 = \pm(3/4)\hbar\Gamma_L(\lambda_L/(2\pi))^3$ is the dispersion coefficient [35–38].

The simulation proceeds through discrete time steps of duration Δt . Before each step, the algorithm determines the

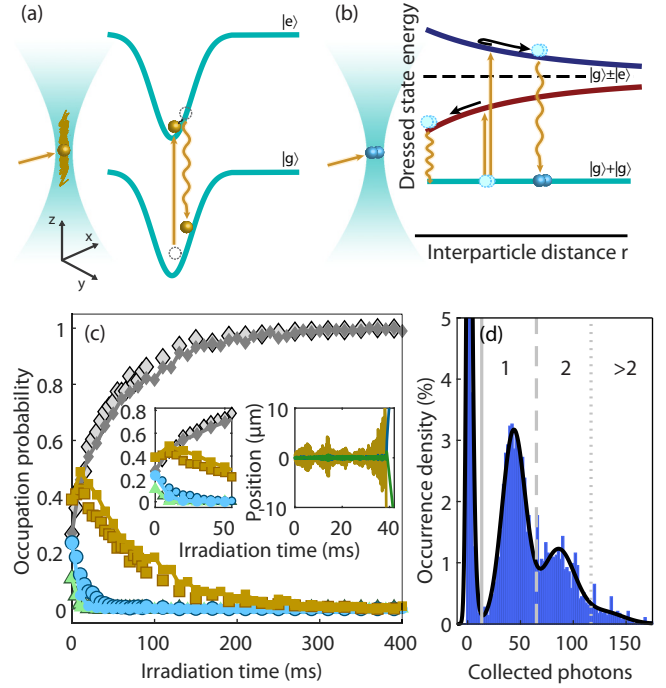


FIG. 1. In-trap population dynamics of few erbium atoms under horizontal yellow-light irradiation. (a) Single-atom scattering via absorption and emission, leading to recoil heating. (b) Two-atom LACs, coupled to dressed states with attractive (red) or repulsive (blue) resonant DDI. (c) Evolution of trap-occupation probability for 0 (diamonds), 1 (squares), 2 (circles), and >2 atoms (triangles). Each point is an average of 200 runs, and error bars reflect uncertainties according to binomial classification with one standard deviation confidence intervals. Solid lines show MC simulations initialized from experimental populations. Left inset: Close-up into the initial 50 ms of time evolution of in-tweezer population. Right inset: Atom trajectory $\mathbf{r}_i = (x, y, z)$ in a single exemplary run (colors: x , blue; y , green; z , yellow). (d) Number-resolved ultrafast imaging after a 7 ms LACs pulse. The histogram shows about 3000 repetitions. For panels (c) and (d), the yellow light has $\Delta_h = -1.2\Gamma_L$, $s_{0,h} = 0.64$, with tilt angle $\theta_h \approx 11^\circ$ to the x - y plane. Gravity points along $-z$.

presence or absence of each ground-state atom by evaluating the sum of the trapping potential and kinetic energy, $E_i = V_{\text{tw}}(\mathbf{r}_i) + m|\mathbf{v}_i|^2/2$. If $E_i > 0$, the atom escapes the trap and is removed from the simulation. Next, the algorithm randomly decides with probability $P_{i,q} = R_{\text{scatt}}(s_{0,q}, \Delta_{i,q}) \times \Delta t$ if an atom gets excited. If no atom is excited, we integrate Eq. (1) for Δt , setting $V_{\text{int}}(r) = 0$. Otherwise, we integrate the equation for a duration accounting for the excited-state lifetime τ_e , which is randomly drawn from an exponential distribution and $V_{\text{int}}(r) \neq 0$. We note that C_3 can be either positive or negative because of the exchange symmetrization [30]. The algorithm samples the sign stochastically, taking into account the different photon excitation probability due to the additional energy shift $V_{\text{int}}(r)$. To account for recoil, the atom's velocity is updated at the start and end of the excited-state interval as $\mathbf{v}_i \rightarrow \mathbf{v}_i + \hbar\mathbf{k}_{\text{rec}}/m$, with $\mathbf{k}_{\text{rec}} = \mathbf{k}_q$ for absorption and $\mathbf{k}_{\text{rec}} = k_L\hat{u}$ for spontaneous emission, where $\hat{u}$ is a unit vector randomly drawn to match the dipolar emission

pattern for σ transitions. This process is repeated until either the final illumination time is reached or all atoms are lost.

III. RESULTS

From the simulation, we obtain the full trajectories of up to three atoms along with the total number of scattered photons. The simulated atom-number-resolved time evolution can be directly compared to experimental data, as our previously demonstrated ultrafast fluorescence imaging technique [12] allows for resolution of individual atom numbers with exposure times short enough (a few microseconds) to freeze the system dynamics during detection [12,39,40]. Moreover, we verify that imaging with the trap on or off yields identical results within our experimental sensitivity (see Ref. [28]). This enables a one-to-one benchmarking of theory and experiment without the need for model-based postprocessing or indirect inference. To initiate this comparison, we perform a first experimental survey—similar in spirit to Ref. [12]—by loading three to four atoms into the tweezer from the MOT and irradiating the sample with a single yellow beam ($q = h$) for a variable time to drive LACs.

From the collected photons, we construct the corresponding histogram and extract the number of trapped particles using the technique of threshold identification [12]. Figure 1(d) depicts a classification into 0, 1, 2, and >2 atoms with thresholds marked with vertical gray lines. We note, however, one key difference with our previous experiment: We use a tweezer wavelength of $\lambda_{\text{tw}} = 486$ nm, 2 nm shorter than in Ref. [12]. This small shift significantly improves atom lifetime during LACs by suppressing detrimental two-photon excitations [11], driven by the sum of the yellow and the tweezer light (see Ref. [28]).

Figure 1(c) exemplarily shows our experimental results together with the MC simulations. In great agreement with each other, both theory and experiments clearly reveal the action of both pair ejection and recoil heating on the in-trap population. Indeed, the probabilities that two and more particles occupy the tweezer rapidly decrease with the irradiation time due to LACs. The probability of single-atom occupation instead increases, reaching a maximum close to 50% after about 20 ms. It then gradually declines, ultimately leading to an empty trap. This latter behavior is due to the recoil heating, which progressively drives the remaining atom out of the trap. Our MC model, initialized following the experimental conditions, reproduces remarkably well the observed in-trap dynamics at both short and long times without the need of any fitting parameters, confirming the predictive power of the model and allowing to quantify the detrimental impact of the recoil heating in maintaining single-atom occupancy [11,26,41,42]. The right inset shows an exemplarily time trajectory of the atom's position in the tweezer, which is spreading due to the recoil heating.

We now use the same MC model as an exploratory tool to identify effective strategies for mitigating the recoil heating in lanthanides. By performing a systematic variation of key parameters—such as intensity, detuning, and quantity of near-resonant yellow beams, as well as tweezer-trap properties—we find a parameter regime for which the simple addition of a second vertically propagating yellow beam

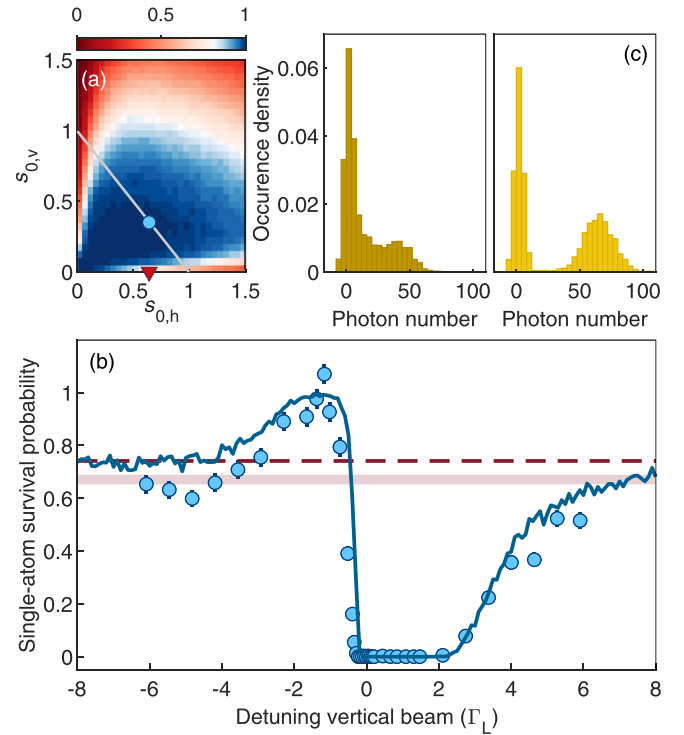


FIG. 2. Effect of axial cooling on the single-atom survival. (a) Calculated two-dimensional intensity map $s_{0,q} = (s_{0,h}, s_{0,v})$ of the single-atom survival probability. In the color scale, we choose white as the color identifying 80% survival probability. Colored markers indicate the parameters used in panel (b): circles for $s_{0,q} = (0.64, 0.35)$ and triangles for $s_{0,q} = (0.64, 0)$. The gray line corresponds to $R_{\text{scatt}} = 75 \times 10^3 \text{ s}^{-1}$. (b) Single-atom survival vs Δ_v , with (circles, solid line) and without (band, dashed line) vertical cooling. Markers and bands show experimental data, whereas lines represent theoretical data. (c) Single-atom histograms obtained with the narrow-line imaging for $s_{0,v} = 0$ (left) and $s_{0,v} = 0.5$ (right), with 40 ms of exposure time and $\Delta_{h,v} = -1.0 \Gamma_L$, taken with 5600 repetitions. Error bars in panel (b) reflect one-sigma standard errors including propagated errors from LACs efficiency and survival. Number of MC runs and initial conditions as in Fig. 1. In panels (a) and (b), $\Delta_h = -1.2 \Gamma_L$; in panels (a) and (c), $\Delta_v = -1.2 \Gamma_L$, and the illumination time is 30 ms. More experimental details can be found in Ref. [28].

($q = v$) provides enough axial Doppler cooling to counteract the recoil heating, substantially increasing the single-atom survival. To illustrate this result, we focus on the one-body scattering dynamics by initializing the system with a single atom in both the simulations and experiment. For the latter, we use a preceding LACs stage. We then study recoil heating with and without the vertical yellow beam applied.

Figures 2 (a) and 2(b) summarize our results. In panel (a), we compute a two-dimensional map of the single-atom survival probability, as a function of the horizontal and vertical yellow beam intensities. The blue region highlights high single-atom survival, which may be combined with large scattering rate for an optimal parameter regime, in which unit survival is never reached in the absence of—or for overly strong—vertical illumination. Moreover, we observe that the effectiveness of vertical cooling depends strongly on its

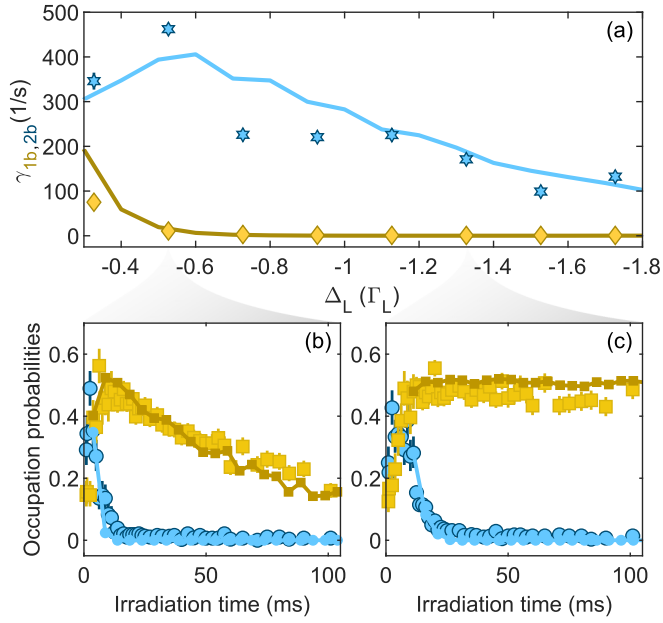


FIG. 3. Light-assisted collisions as a function of detuning. (a) Two-body LACs rate (blue) extracted from time trace of the occupation probability as a function of the illumination time [panels (b) and (c)] by fitting the curves with a rate equation and an exponential decay (see Ref. [28] for more details). For comparison, the one-body loss rate due to recoil heating is also shown (yellow). In panels (b) and (c), the detunings of the yellow light are $\Delta_L \approx -0.5 \Gamma_L$ and $\Delta_L \approx -1.3 \Gamma_L$, respectively. For all the plots, $s_{0,q} = (0.64, 0.39)$.

detuning, as shown in panel (b). Notably, we identify a sizable red-detuning window around $-1 \Gamma_L$ where the survival probability reaches unity, indicating a favorable regime for low-loss operation. The MC simulation captures both the qualitative trend and the resonance position in good agreement with the experiment. Away from resonance, the survival probability returns to a background level, matching the value observed in the absence of the vertical beam. We also observe that the axial cooling plays a key role for continuous imaging, a feature which is essential in operating reconfigurable tweezer arrays. Figure 2(c) exemplarily shows this effect for the yellow imaging, where we see that the fidelity increases from $93.6^{+1.8}_{-2.5}\%$ without cooling to $99.96^{+0.03}_{-0.24}\%$ with cooling [43].

The promising results presented above enable us to disentangle and suppress the effects of recoil heating from the LACs dynamics, thereby allowing us to address the central question of single-atom preparation efficiency. We repeat the measurement of the number-resolved population dynamics of Fig. 1(c), but now adding the axial cooling beam, and extract the two-body LACs rate, γ_{2b} . As shown in Fig. 3(a), γ_{2b} has a nonmonotonic behavior, showing a maximum at $\Delta_L \approx -0.5 \Gamma_L$ [Fig. 3(b)], followed by a slow decrease. For detunings smaller than $\Delta_L \approx -0.7 \Gamma_L$, we find an optimal situation in which LACs-induced pair projection is efficient and one-body losses due to heating (γ_{1b}) are negligible [Fig. 3(c)]. Together with the data, we also show the results of our Monte Carlo algorithm (solid lines), which agree remarkably well with the observations, confirming again the model as an exceptional tool for reproducing and predicting the physics at play.

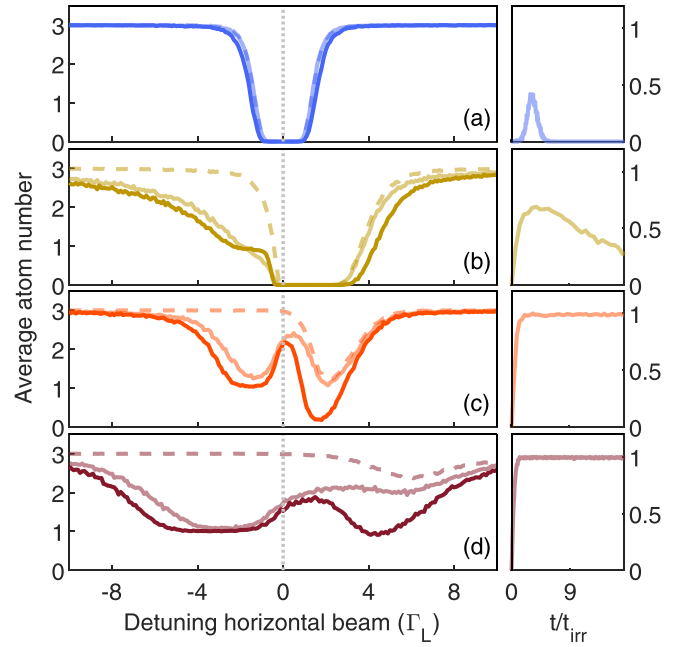


FIG. 4. Single-atom preparation efficiency. Left side: Panels (a)–(d) depict the average atom number vs light detuning, for the blue ($\lambda_L = 401$ nm, $\Gamma_L/(2\pi) = 28$ MHz), the yellow, the orange ($\lambda_L = 631$ nm, $\Gamma_L/(2\pi) = 28$ kHz), and the red ($\lambda_L = 841$ nm, $\Gamma_L/(2\pi) = 8$ kHz) transitions, respectively, with $s_{0,q} = (1.00, 0)$ (solid, light color) and $s_{0,q} = (1.00, 0.55)$ (solid, dark color), during an irradiation time t_{irr} (see main text). In panel (b), we consider $20 \times t_{irr}$ in order to highlight the effect of axial cooling. The dotted line marks $\Delta_h = 0$, and the dashed lines correspond to simulations without DDI. Right side: Evolution of one-atom trap-occupation probability for the detuning corresponding to the minimum of the LACs feature, with $s_{0,v} = 0$ and $\Delta_L/\Gamma_L = 0, -0.5, -1.4$, and -2.8 for the blue, yellow, orange, and red transitions, and the corresponding $t_{irr} = 2.4 \mu s, 0.76$ ms, 5.9 ms, and 36 ms. We multiply the x axis of the right side of panel (a) by 0.1 .

We use the predicting power of our MC algorithm to explore the performance of single-atom preparation for different lanthanide transitions. In particular, we test the interplay between LACs and recoil heating for four different lines—blue, yellow, orange, and red—spanning linewidths from tens of megahertz to a few kilohertz. For all simulations, we illuminate the atoms for a time t_{irr} with a single horizontal beam of intensity $s_{0,h} = 1$. Because of the largely different transition strengths, we rescale the irradiation time according to $t_{irr} = U_0/(E_{rec} \Gamma_L)$, where U_0 is the trap depth and E_{rec} is the recoil energy associated with the different transitions.

Figure 4 summarizes our results. For each transition, we plot the average number of atoms remaining after irradiation as a function of the light detuning. Assuming an initial state of three atoms, we perform simulations with and without vertical cooling. For the latter case, we also perform simulations without C_3 and hence LACs. In general, we observe two distinct features: a recoil-heating minimum on the blue-detuned side and a LACs-induced minimum for red detuning. Our simulations reveal that the position and relative strength of these features strongly depend on the transition. This dependence arises not only from the linewidth Γ_L but also from the laser

wavelength λ_L [35], and is further amplified in lanthanides, where the linewidth typically decreases with increasing wavelength [44]. For the strong blue transition, the two minima overlap, and the dynamics are dominated by recoil heating [panel (a)], regardless of the presence of a vertical beam. As we move to narrower transitions [panels (b)–(d)], the minima become more distinct, with the red line [panel (d)] exhibiting the greatest contrast. Here, while the vertical beam counteracts the recoil heating for the yellow transition (see also Ref. [28] for results with our experimental parameters), it is not required for the orange and red ones. Notably, this red transition also shows signs of blue-detuned LACs, as evidenced by the difference in minimum depth between the full simulation and the one accounting only for recoil heating.

In tweezer-based architectures, not only single-atom fidelity is crucial, but also the preparation time [28], especially for gate-based applications. The right panels of Fig. 4 display the time evolution for each transition, which, as expected, is slower for narrower lines. In single-beam experiments, the orange transition—unique to lanthanides and not available in Sr or Yb—strikes a favorable balance between fidelity and speed. As demonstrated in our yellow-line experiment (see Fig. 3), this performance could be further enhanced using an additional cooling beam.

IV. CONCLUSION

In summary, we have developed and validated a Monte Carlo simulation framework to model the dynamics of erbium atoms trapped in optical tweezers under near-resonant illumination. Our approach accurately reproduces experimental observations of single- and two-body processes, including recoil heating and light-assisted collisions, without relying

on fitting parameters. The simulations identify optimal conditions for single-atom retention and reveal how different optical transitions can be selectively leveraged for efficient preparation. In particular, we clearly distinguish the roles of light-assisted collisions and recoil heating, uncovering regimes where these effects are well separated. These findings not only deepen our understanding of atom-light interactions in lanthanide tweezer arrays but also establish a powerful theoretical framework for designing next-generation quantum experiments with strongly magnetic atoms.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [45].

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