Controlling cold atom-ion collisions using a Rydberg state

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We present a method to control the cold collision between an ultracold atom and a trapped ion. A laser is used to excite the ground state atom to a repulsive Rydberg potential level at a certain atom-ion distance. In this way the ion is effectively surrounded by a potential wall that the atom cannot cross. Once the atom leaves the interaction area, it is de-excited back to its original level. The adiabaticity of the scheme is analyzed as a function of different parameters such as laser frequency, laser power, the initial atom-ion collision energy, as well as the direction of the collisional process with respect to the light field. By controlling e.g. the laser power and the laser frequency, as well as by addressing different Rydberg states, the properties of this shielding effect can be widely tuned. In particular, unwanted chemical reactions between atoms and ion can efficiently be suppressed, which is an important step towards realization of diverse quantum technological applications for hybrid atom-ion systems.

I. INTRODUCTION

The developing field of hybrid systems of cold, trapped atoms and ions (for a review see, e.g., [1–3]) has brought forth a number of proposals for novel experiments. For a majority of these, such as studies of polarons in strong coupling regimes [4], formation of mesoscopic molecular ions [5], realization of artificial solid state physics systems [6], demonstration of switches for atomic motion [7], and implementation of atom-ion quantum gates [8], reactions between atom and ion are unwanted and need to be suppressed.

One way to prevent atom and ion from reacting with each other is by keeping them at a safe distance by tightly trapping them individually [9]. Another approach is optical shielding which has been introduced about twenty years ago as a tool to reduce inelastic losses in samples of ultracold neutral atoms [10–12]. Here, a blue-detuned laser induces a transition of one of the colliding atoms to a repulsive electronically excited state. During the excitation the atoms repel each other which prevents a further approach of the particles. Collisional suppressions of up to a factor of 30 have been demonstrated [13]. Recently, the emergence of cold molecules has stimulated a renewed interest in optical shielding [14–16]. These proposed schemes rely on Rydberg-dressing, i.e. laser-admixing of Rydberg levels to the ground states taking advantage of the corresponding large electrical dipole moments. Rydberg-dressing was also recently proposed for shielding the collision between an ultracold neutral atom and an ultracold ion [19]. Here, Rydberg dressing operates on a per se forbidden $S$ to $S$ transition. However, as the particles approach each other, the electrical field of the ion increasingly admixes $P$-states to the Rydberg $S$-level, which increases the optical coupling to the Rydberg $S$-level and creates an increasing repulsive ac-Stark-shift potential.

In this work, we propose a somewhat different optical shielding scheme for an atom-ion collision which is based on an adiabatic optical transition of the ground state atom to a low-field seeking Rydberg state and back. We analyze the efficiency of the shielding process as a function of laser frequency, laser power, the initial collision energy and the relative orientation of the colliding particles with respect to the laser field.

II. GENERIC SHIELDING SCHEME

We consider an atom in the electronic ground state $|g\rangle$ which collides with a trapped ion in a two-body collision, see Fig. 1. The ion is located in an intense continuous wave laser field. The distance between atom and ion is denoted $r$. When $r$ reaches the shielding distance $r_s$, the atom is resonantly excited to a Rydberg state $|e\rangle$ by the laser field. The Rydberg state has a large low-field seeking electrical dipole moment which leads to a repulsion of the collision partners, such that the atom is effectively reflected off a potential wall at distance $r_s$. After the reflection the atom is adiabatically de-excited back to the ground state. The collision takes place within a time scale which is much shorter than the natural lifetime of several $\mu$s of the Rydberg state. Therefore spontaneous radiative decay of the Rydberg atom is negligible.

We now estimate the shielding efficiency of this scheme with the following simple two-channel model, where we e.g. neglect interactions between the ground state atom and the ion. Furthermore, we assume that the atom-ion collision takes place in an s-partial wave, and that the laser coupling between the atomic ground and Rydberg state is isotropic. Using the rotating wave approximation the interaction Hamiltonian in the rotating frame is

$$V_I = \left( \begin{array}{cc} V_0 & \frac{\hbar \Omega}{2} \int (r-r_s) \, dV_e/dr \, dr \end{array} \right),$$

\[1\]
FIG. 1: Blue shielding scheme using a Rydberg level. In a collision a neutral ground state atom approaches an ion. At a distance \( r \approx r_s \) a cw laser excites the neutral atom to a Rydberg level. The Rydberg atom is in a low-field seeking state and is strongly repelled by the electric field of the ion. Effectively, the atom is reflected from a potential shield around the ion. As the reflected atom leaves it is de-excited to the ground state by the laser in an adiabatic fashion.

where the uncoupled ground state channel \(|g\rangle\) has a constant potential energy \( V_g \) which we arbitrarily choose to be zero, \( V_g = 0 \). The potential energy of the low-field seeking Rydberg channel, on the other hand, has a constant slope \( dV_e/dr \), as depicted in Fig. 2(a). The coupling \( \Omega \) of the two channels leads to an avoided crossing around \( r_s \). If for a given atom-ion collision energy \( E_{coll} \) the atom passes the avoided crossing adiabatically it will climb the potential slope of the Rydberg state \(|e\rangle\) until it turns around and is reflected back to where it came from. In order to obtain quantitative results, we solve the radial Schrödinger equation

\[
\left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_I(r) \right) \Psi = E_{coll} \Psi. \tag{2}
\]

Here, \( \mu \) is the reduced mass of the colliding system of atom and ion and \( \Psi = (\varphi_g, \varphi_e)^T \) is a two-component wavefunction. We are looking for scattering solutions for this one-dimensional problem where the only incoming probability flux towards the avoided crossing is in the ground state channel (coming in from large \( r \)). The Schrödinger equation is numerically integrated for a chosen collision energy \( E_{coll} \) as described in the appendices A and B. In order to calculate the incoming and outgoing flux in each channel at sufficiently large distances from \( r_s \) we locally express each wavefunction component \( \varphi_{e,g} \) in terms of \( ae^{ikr} + be^{-ikr} \) with \( k = \sqrt{2\mu E_{coll}/\hbar} \). The amplitudes \( a, b \) are determined using \( a = (\varphi_g' + ik \varphi_e)/(2i\varphi_e e^{ikr}) \) and \( b = (\varphi_g' - ik \varphi_e)/(-2i\varphi_e e^{-ikr}) \), respectively. Here, \( \varphi'_g \) denotes the derivative \( \varphi'_g = d\varphi_g/dr \). The fraction of the probability density being reflected at the blue shielding potential wall is then given by \( |a|^2/(|a|^2 + |b|^2) \). This fraction is plotted in Fig. 2(b) as a function of a scaled coupling strength

\[
\bar{\Omega} = \hbar \Omega \left( \frac{2\mu}{\hbar^2 E_{coll}} \right)^{1/4} |dV_e/dr|^{-1/2} \tag{3}
\]

for a collision energy \( E_{coll} = 1\text{mK} \times k_B \) and several slopes \( dE_e/dr \) (see legend). We note that in a range of reflection probabilities between about 10 and 90% all curves for the different slopes \( dE_e/dr \) are quite similar. They
can therefore approximately be described by a universal function. We find that e.g. a function of the form \( P_r(\Omega) = 1 - \exp(-2.4\Omega^2/5.4 + \Omega^2) \) fits reasonably well in the given range (see black solid line in Fig. 2(b)). For comparison, the red dashed line shows the reflection probability when simply applying the Landau-Zener formula \( P_r^{LZ} = 1 - \exp(-\pi\Omega^2/4) \) [20, 21]. 

1 - \( P_r \) is the probability for a non-adiabatic transition through the avoided crossing. Here, the shielding does not work, since either the particles will collide at short distance or they will fly apart in an accelerated way, converting the potential energy of the \( V_e \) level into kinetic energy.

A possible candidate for Rydberg shielding as described is \(^{23}\text{Na}\). Figure 3(a) shows a Stark map of the \( n = 14 \) hydrogen-like manifold as well as the \( n = 17 \) \( P \)-level which is a low-field seeker. Here, \( n \) denotes the principal quantum number. The \( 17 P \)-level has a natural lifetime of about 5 \( \mu s \) (incl. decay due to BBR) [22]. By appropriately choosing the laser frequency a convenient slope \( dv_e/dr \) can be chosen. To convert the electrical field \( E_f \) on the \( x \)-axis into the internuclear distance \( r \) we can approximately [28] make use of \( E_f = \varepsilon/4\pi\varepsilon_0 r \), assuming that the ion is singly charged. Here, \( \varepsilon \) is the elementary electric charge, and \( \varepsilon_0 \) is the dielectric constant of the vacuum. As an example for possible shielding parameters for \(^{23}\text{Na}\) we choose a laser which resonantly excites the Rydberg state at -420 cm\(^{-1}\) and is thus blue detuned by 1 cm\(^{-1}\) from the \( 17P \) state at zero field (see Fig. 3(a)). Resonant Rydberg excitation occurs then at a distance of about 200 nm where the gradient \( dv_e/dr \) is about \( \approx 0.6 \text{ GHz/nm} \times \hbar \). For a Rabi frequency \( \Omega = 2\pi \times 400 \text{ MHz} \) we obtain a scaled coupling strength \( \Omega \approx 2 \) which according to Fig. 2(b) corresponds to a reflection efficiency larger than 90%.

The situation gets more complicated, but also more interesting, when considering atomic species with high-field seeking \( P \)-states, such as \(^{87}\text{Rb}\). The Stark map for \(^{87}\text{Rb}\) is shown in Fig. 3(b). (We note that for \(^{87}\text{Rb}\) the \( 17P \) level is split up into two fine structure components with a total electronic angular momentum of \( j = 1/2 \) and \( 3/2 \)). Obviously, high-field seeking states would normally be inappropriate for Rydberg shielding with our scheme. Nevertheless, even here shielding can still be achieved by making use of an avoided crossing of a \( P \)-level with a level of the \( n = 14 \) hydrogen-like manifold. Fig. 3(b) shows several of such avoided crosses in the region which is marked in light blue. Close to the shown avoided crossings there is a substantial admixing of \( P \)-character to the levels of the hydrogen-like manifold which are low-field seeking. Therefore, via this admixture electric dipole transitions between the atomic ground state \( |g\rangle \) and these low-field seekers are possible.

In the following we will study in detail how Rydberg shielding works right at the tips of these avoided crossings. In Fig 3(b) the first avoided crossings occur at an electrical field of about 2100 V/cm. This corresponds to a reflection distance \( r_s \) of about 80 nm. In order to resonantly couple to these avoided crossings, a laser wave-

\[ |g\rangle \rightarrow |e\rangle \]

\[ \text{length of about 301.7 nm is needed.} \]

In principle, \( r_s \) can be tuned over a large range by choosing an appropriate avoided crossing, e.g., in another manifold with a different \( n \) quantum number. We find that \( r_s \approx 0.079 \text{ nm} \times n_{eff}^{2.59} \), where \( n_{eff} = n - \delta(n) \) is the effective quantum number and \( \delta(n) \) is the quantum defect [29]. For the \( n \)-quantum numbers between 13 and 26, the shielding radius \( r_s \) ranges from 33 to 269 nm.

\[ \text{FIG. 3: (a) Stark spectrum of } ^{23}\text{Na} \text{ in the vicinity of the low-field seeking } 17P \text{ state. (b) Stark spectrum of } ^{87}\text{Rb} \text{ in the vicinity of the high-field seeking } 17P \text{ state. At avoided crossings (cyan colored area) } 17P \text{ state character is admixed to low-field seeking states of the } n = 14 \text{ level manifold.} \]

\[ \text{III. A CASE STUDY} \]

In the previous section we have briefly sketched the physics behind Rydberg shielding which involved a number of simplifications and assumptions. We now proceed...
A. Ground state polarization potential, centrifugal barrier and collision energy

In Eq. (1) we have neglected the interaction potential \( V_g \) between ground state atom and ion. The long-range tail of \( V_g \) (see e.g. ref. [1]) is given by

\[
V_g(r, l) = - \frac{C_4}{2r^4} + \frac{k^2(l+1)}{2\mu r^2},
\]

where the first term represents the polarization potential and the second term is the centrifugal potential barrier. Here, \( C_4 = \hat{\alpha}\varepsilon^2/(4\pi\varepsilon_0) \) and \( \hat{\alpha} = 4.73 \times 10^{-29} \text{ m}^3 \) is the static electric dipole polarizability of the neutral \(^{87}\text{Rb}\) atom in the electronic ground state \( 5S_{1/2} \) [22]. \( l \) is the quantum number of the partial wave.

In current experiments, the collision energy of a cold ion in a Paul trap colliding with an ultracold atom is typically on the order of \( 1 \text{ mK} \times k_B \), due to effects of micromotion of the ion. This is indeed much larger than the \( \approx 10 \mu\text{K}\times k_B \) depth of the polarization potential at the shielding distance \( r_s \approx 80 \text{ nm} \). Therefore, the polarization potential in the ground state can be safely neglected.

At the same shielding distance \( (r_s \approx 80 \text{ nm}) \) the centrifugal barrier reaches a height of \( 1 \text{ mK} \times k_B \) for \( l = 38 \). Therefore, a large number of partial waves are involved in a typical atom-ion shielding experiment. Nevertheless, if shielding works for the \( s \)-wave it will also work for the higher partial waves because the centrifugal barrier only helps the shielding. Therefore, we can quite generally restrict ourselves to the discussion of only the \( s \)-wave. Doing so, we neglect mixing of partial waves, which occurs because the atom-ion interaction is in general not spherically symmetric. However, this mixing is not relevant for shielding and therefore beyond the scope of this work.

Finally, we would like to mention that besides resonantly coupling the ground state and the Rydberg state the shielding laser also produces an optical dipole potential for Rydberg state atoms. We have calculated the dipole potential to be repulsive and to be around \( 600 \mu\text{K}\times k_B \) for the typically needed laser intensities of our shielding scheme [23]. Since this is of the order of the collision energy it needs to be considered in the setting up of a real experiment. In principle the repulsive dipole potential can be compensated by applying an additional attractive dipole trap, e.g. based on a high-power 1064 nm polarized laser.

B. Interaction between Rydberg atom and ion

In section [11] the interaction between Rydberg atom and ion was approximated at several instances. We will now improve the treatment. In particular, we will take into account the inhomogeneity of the electrical field of the ion. The field of the ion polarizes the Rydberg atom by mixing various orbital angular momentum states. This turns the Rydberg atom into an electric multipole which is either attracted or repelled by the ion. For the calculations it is convenient to use a multipole expansion [20] of the Rydberg electron-ion interaction. For now, let the Rydberg nucleus be located at the origin of the coordinate system and the ion on the \( z \)-axis at a distance \( r \). The potential of the ion in the multipole field of the electron is then given by

\[
V_{e,\text{ion}} = \frac{e}{4\pi\varepsilon_0} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} Y_{lm}(0,0) q_{lm} = \frac{e}{4\pi\varepsilon_0} \sum_{l=0}^{\infty} \sqrt{\frac{4\pi}{2l+1}} \frac{1}{r^{l+1}} q_l, \tag{5}
\]

where we have used that \( Y_{lm}(0,0) = \delta_{m,0} \sqrt{(2l+1)/4\pi} \) and \( q_l \) are the spherical multipole moments of the Rydberg electron. For an electron located at the position \((r_e, \theta_e, \phi_e)\) in spherical coordinates, \( q_l \) is given by

\[
q_l = -e r_l^2 Y_{lm}^*(\theta_e, \phi_e). \tag{6}
\]

When viewed in terms of operators, the \( q_{lm} \) components with \( l > 0 \) are responsible for the mixing of different orbital momenta of the Rydberg atom. If we add to \( V_{e,\text{ion}} \) the repulsion between the Rydberg ion core and the ion, \( V_{\text{ion,ion}} = e^2/(4\pi\varepsilon_0 r^2) \), we finally obtain for the total interaction,

\[
V_{e+\text{ion,ion}} = -\frac{e^2}{4\pi\varepsilon_0} \sum_{l=1}^{\infty} \sqrt{\frac{4\pi}{2l+1}} \frac{r_l^2}{r^{l+1}} Y_{lm}^* (\theta_e, \phi_e). \tag{7}
\]

The lowest-order term in Eq. (7) corresponds to \( l = 1 \) and treats the atom-ion interaction as if the electrical field produced by the ion were homogeneous at the location of the atom. It gives rise to the Stark effect in homogeneous fields, as in Fig. [3]. In our calculations we truncate the sum in Eq. (7) to include only terms up to \( l = 6 \), since higher order terms lead to negligible contributions. Using the Born-Oppenheimer approximation we obtain effective potential energy curves \( V_e(r) \) between Rydberg atom and ion (see e.g. Fig. [3]) by solving the Schrödinger equation for the electron motion,

\[
(H_0 + V_{e+\text{ion,ion}}) \Psi_e = V_e(r) \Psi_e. \tag{8}
\]

Here, \( H_0 \) is the unperturbed Hamiltonian of the Rydberg atom and \( \Psi_e \) is the electronic wavefunction of the Rydberg atom.

Figures [4] (a) and (b) present numerical calculations of \( V_e(r) \) for \(^{87}\text{Rb}\), again for the hydrogen-like \( n = 14 \) manifold, together with the fine structure split levels \( P_{3/2} \) and \( P_{1/2} \) of \( n = 17 \). The fine structure splitting also leads to a (much smaller) doublet structure of the \( n = 14 \) manifold. Shown are the results for magnetic quantum numbers \( m_J = \pm 3/2 \) (a) and \( m_J = \pm 1/2 \) (b) of the Rydberg atom with total angular momentum \( J \).
where the $P_{3/2}$ component of the Rydberg wavefunction is positive. Then we find that for the energetically degenerate states $|e, \pm m_j\rangle$ and $|g, \pm m_j\rangle$ we have

\[ \langle e, m_j' | e r_{e,i} | g, m_j \rangle = \langle e, -m_j' | e r_{e,-i} | g, -m_j \rangle, \]

i.e. $d_{el,i} = d_{el,-i}$.

As expected, the transition matrix elements $d_{el}$ vary markedly at the avoided crossings as a consequence of mixing between the $17P$ and the hydrogen-like orbitals.

The transition dipole moment $d_{el}$ together with the electrical light field $E$ determine the Rabi frequency $\Omega$ for the coupling of $|g\rangle$ and $|e\rangle$, see also Eq. (10). $\Omega$ is defined by

\[ \frac{\hbar \Omega}{2} = \sum_i \mathcal{E}_i d_{el,i}, \]  

where $\mathcal{E}_i (i \in \{+1, 0, -1\})$ are the spherical components ($\sigma^+, \pi, \sigma^-$) of the light field.

We now consider the internuclear axis to have an angle $\theta$ with the quantization axis $z$ which is defined by the propagation direction of the laser, see Fig. 1 and appendix E. In the $\{x', y', z'\}$-frame the internuclear axis is the quantization axis ($z'$-axis). In this primed frame the atomic ground state $|g\rangle = \sum_i \beta_i |g, m_i\rangle$ becomes $|g'\rangle = \sum_i \beta_i' |g, m_i\rangle$ and the spherical light field components $\mathcal{E}_i$ become $\mathcal{E}_i'$. Thus the Rabi frequency becomes

\[ \frac{\hbar \Omega}{2} = \sum_{i,j} \mathcal{E}_i' \beta_j' \langle e | e r'_{e,i} | g, m_j \rangle. \]

Therefore, in contrast to our previous assumption in section II, $\Omega$ does in general depend on the polar angle $\theta$ (see Fig. 1 and the azimuthal angle $\phi$ (not shown in Fig. 1). In appendix E we show how to calculate $\mathcal{E}_i'$ and $\beta_j'$ (and therefore $\Omega$) with the help of rotational transformations. Furthermore, it is shown that the laser couples the ground state $|g\rangle$ to a well-defined, but angle dependent state $|e_\theta\rangle$ in the resonantly addressed Rydberg manifold which is spanned by the two degenerate states $|e, \pm m_j\rangle$. The decomposition of $|e_\theta\rangle$ into $|e, \pm m_j\rangle$ is given in appendix E.

Figure 2 shows how $\Omega$ changes as a function of the angle $\theta$ for several examples. For these examples we used the dipole matrix elements $d_{el}$ at the tips of the potential curves for the avoided crossings ($C_1, C_{1f}, C_{1II}$), as marked in Fig. 1. These avoided crossings (along with $C_{IV}$) can potentially be used for shielding. How shielding works at the tips will be explained in detail in the next section. Here, we investigate the strength of the shielding and its angular dependence. We chose the laser intensity for all these examples to be the same, $I_L = 40 \text{ mW}/\mu\text{m}^2$.

The magenta continuous line is for a circularly polarized laser which at $\theta = 0$ drives a $\sigma^+$-transition from $|g, m_j = 1/2\rangle$ to $|e, m_j = 3/2\rangle$ at $C_1$. For the given laser intensity $I_L$ the Rabi frequency is $\Omega = 2 \pi \times 1 \text{ GHz}$, which, as we will see in the next section, is a typically required
value for successful shielding. At $\theta = 90^\circ$ the Rabi frequency $\Omega$ has lost half of its initial value at $\theta = 0$. This can be mainly explained by the fact that at $\theta = 90^\circ$ a sizable fraction of the light is $\pi$-polarized and can therefore not drive a transition from the ground state to the $|m_j| = 1/2$ manifold. Nevertheless, it is clear that overall the crossing $C_f$ from the given examples is the best choice in terms of coupling.

The red continuous line is also for a $\sigma^+$-transition, however, to the $|m_j| = 1/2$ manifold at crossing $C_{II}$. Overall, it is weaker than for $C_f$, but it exhibits similar angular dependence. The relative loss at $\theta = 90^\circ$ is somewhat stronger than for $C_f$. This is due to an interference effect where $\sigma$ and $\pi$ transition paths from the rotated ground state, $|g\rangle' = (|g,m_j = 1/2\rangle - |g,m_j = -1/2\rangle)/\sqrt{2}$, to either $|e,m_j = \pm 1/2\rangle$ destructively interfere. In order to make the coupling more isotropic we now try using a linearly polarized laser beam (dashed and dotted red lines) instead of circular polarization. Linearly polarized light is an equal superposition of $\sigma^+$ and $\sigma^-$ light. The polarization direction of the laser light now breaks the rotational symmetry about the $z$-axis (i.e. symmetry in the azimuthal direction $\phi$) which exists for circular polarized light. Therefore, we now analyze the dependence on angle $\theta$ both in the planes perpendicular and parallel to the polarization direction, see horizontal dashed line and dotted line, respectively. Indeed, the dashed line is now flat and therefore $\Omega$ independent on angle. However, in the other plane the anisotropy has somewhat increased. At angle $\theta = 0$ the Rabi frequency $\Omega$ for the dashed and dotted lines is by a factor of $1/\sqrt{2}$ smaller than for circular polarization, i.e. $\Omega_0$, because only one of the two circular components contributes to the coupling towards the $|m_j| = 1/2$ Rydberg manifold.

The green line in Fig. 5 is for $\sigma^+$ laser light coupling to avoided crossing $C_{III}$. For this transition only $\pi$-transitions have sizable $d_{el}$ and $\pi$-component the coupling is maximal.

These examples show that the angular dependence of $\Omega$ can be tuned, e.g. by changing the polarization of the laser beam, making use of interference effects or by addressing different Rydberg states. Additional tuning could be done by using additional laser fields from different directions.

When deciding which of the crossings $C_i$ is best for collisional shielding one also has to consider whether the particles can actually reach the crossing. For example, the $C_f$ crossing is energetically close to the avoided crossing $C_{IV}$ which also exhibits sizable transition matrix elements. Thus, laser coupling to the two curves simultaneously could lead to complications. However, closer inspection shows that at the tip the two potential curves are still split by about 6 GHz$\times$h which should be enough to treat them separately. In order to reach $C_{II}$ the atom has to pass two potential energy curves from the hydrogen-like manifold, see Fig. 4(b). However, because of their small transition matrix elements coupling to these states is negligible. The crossing $C_{IV}$ again looks good in terms of $d_{el}$. In terms of angular dependence it will behave similarly as $C_{II}$. However, in order to reach $C_{IV}$ the atom would have to cross the 17$P_{1/2}$ level (black dashed line) at a distance of about 90 nm. In order to estimate whether the atom might simply non-adiabatically cross, we use the scaled coupling strength $\varpi$ of Eq. (1). While the slope $d\varpi/dr \approx 8$ GHz$\times$h is relatively steep the transition matrix element $d_{el}$ is somewhat larger than for the $C_{IV}$ crossing. Choosing a typical Rabi-frequency $\Omega = 2\pi \times 1$ GHz we obtain a non-adiabatic transmission probability of about 90%. Thus, a dominantly non-adiabatic crossing might work but it is not a clear-cut case. Interestingly, the fraction of the incoming flux which adiabatically gets to be coupled into the 17$P_{1/2}$ state will con-
lead to an anisotropic effective scattering potential between atom and ion. This will cause mixing of different partial waves. However, such a mixing is not of interest here and beyond the scope of this work. In the following we will carry out calculations where we ignore the angular dependence of \( \Omega \), bearing in mind, however, that in order to achieve a target value of shielding the given Rabi frequency might have to be increased by a factor 2 to 3.

IV. NUMERICAL SOLUTION FOR SHIELDING

We now investigate the collision dynamics by numerically solving the Schrödinger equation for the scattering problem. For this, we consider only two coupled channels: (1) The atomic ground state with potential energy \( V_g(r) \), and (2) the atom in a specific excited Rydberg state with potential energy \( V_e(r) \). The two channels are coupled via a laser with the Rabi frequency \( \Omega(r) = d_a(r) \times \sqrt{2I_L/(\epsilon e_0)}/\hbar \), which depends on the relative distance of the atom and the ion. Here, \( c \) is the speed of light and \( I_L \) is the intensity of the shielding laser. As discussed in section IIIC we take the coupling strength to be spherically symmetric. Within the rotating wave approximation, the coupled potentials for the two-level system can be written as

\[
V_I = \left( \begin{array}{cc}
V_g(r) & \hbar\Omega(r)/2 \\
\hbar\Omega(r)/2 & V_e(r)
\end{array} \right),
\]

generalizing Eq. (1). With the new \( V_I \) we numerically solve the Schrödinger equation Eq. (2) using the same method as before, see appendices A and B. Here, the two components of the wavefunction are denoted by \( \varphi_U \) and \( \varphi_L \), where the subscript indicates the energetically lower branch (\( L \)) and the energetically upper branch (\( U \)), respectively. The task is to calculate scattering solutions for flux entering from large internuclear distance in channel \( U \). This flux can then be reflected, transmitted, or it can non-adiabatically leak into channel \( L \).

Figure 6(a) shows an example for the resulting potential curves \( V_U, V_L \) (solid lines) as well as the uncoupled energies \( V_g, V_e \) (dashed lines), corresponding to the avoided crossing \( C_{II} \) of Fig. 4(b). The laser frequency is chosen such that \( V_g \) intersects the potential barrier \( V_e \) 500 MHz \( \times \) 1 below its tip. This setting corresponds to a detuning \( \Delta = -2\pi \times 500 \) MHz. We choose a laser intensity of 158 mW/(2\( \mu \)m)\(^2\) which corresponds to a maximal Rabi frequency of \( \Omega_{\text{max}} = 2\pi \times 730 \) MHz at \( r = 72.3 \) nm. We choose a collision energy of \( E_{\text{coll}} = 1 \) mK \( \times k_B \). \( j_1, j_2, j_3 \) is the incoming, reflected and transmitted currents, respectively. \( j_1 \) and \( j_2 \) are the currents that non-adiabatically leak into channel \( V_L \). (b) Real parts of the calculated scattering wavefunctions \( \varphi_U \) (black solid line) and \( \varphi_L \) (red solid line). (c) and (d) are calculations using the same parameters as in (a) and (b), except that \( \Delta = 2\pi \times 500 \) MHz.

As shown in Fig. 6(a), we label the incident current as \( j_i \), the reflected current as \( j_r \), the transmitted current as \( j_t \) and the currents non-adiabatically leaking to the \( L \)-channel as \( j_1 \) and \( j_2 \). For the example (a), \( j_r/j_t = 52\% \) of the incident current is reflected, \( j_1/j_t = 3\% \) is transmitted (mainly by tunneling) and \( (j_1 + j_2)/j_t = 45\% \) is lost to channel \( L \). For the example (c), \( j_r/j_t = 71\% \) of the incident current is reflected, \( j_1/j_t = 7\% \) is transmitted and \( (j_1 + j_2)/j_t = 22\% \) is lost to channel \( L \). Thus, a detuning \( \Delta > 0 \) leads to better shielding. The parameters for the two examples discussed here have been chosen so that there is still a sizable tunneling and leakage current, for the sake of the discussion. We will

\[
\begin{align*}
& V_U = \left( \begin{array}{cc}
V_g(r) & \hbar\Omega(r)/2 \\
\hbar\Omega(r)/2 & V_e(r)
\end{array} \right), \\
& j_i, j_r, j_t, j_1, j_2, j_3,
\end{align*}
\]

(c) are shown in plots (b) and (d), respectively. The distortion of the wavefunctions \( \varphi_U \) at around \( r = 74 \) nm indicates that the non-adiabatic coupling takes place in the direct vicinity of the avoided crossing, as expected. Furthermore, it is already clear to see that the amplitude for \( \varphi_U \) is smaller on the left hand side of the barrier than on the right hand side. This is a first indication for shielding, which we will now quantify by comparing incoming, reflected and leaking probability currents. For this, we locally (far enough away from the barrier) express the scattering wavefunctions for each scattering channel (\( q \in \{U, L\} \)) in terms of \( \varphi_q = a_q e^{i k_q r} + b_q e^{-i k_q r} \), similarly as described in section IIIC. From this we can extract the local currents \( |a_q|^2 k_q \hbar/\mu \) and \( |b_q|^2 k_q \hbar/\mu \), where \( k_q = \sqrt{2\mu(E_{\text{coll}} - V_q(r))/\hbar} \).

FIG. 6: (a) Calculated potential energies with coupling (\( V_U \) and \( V_L \), solid lines) and without coupling (\( V_e \) and \( V_g \), dashed lines) for \( \Delta = 2\pi \times 500 \) MHz, \( \Omega_{\text{max}} = 2\pi \times 730 \) MHz and \( E_{\text{coll}} = 1 \) mK \( \times k_B \). (b) Real parts of the calculated scattering wavefunctions \( \varphi_U \) (black solid line) and \( \varphi_L \) (red solid line). (c) and (d) are calculations using the same parameters as in (a) and (b), except that \( \Delta = 2\pi \times 500 \) MHz.
show further below that the shielding efficiency can be nearly 100% by increasing the coupling strength \( \Omega \) by a mere factor of 2.

Besides the reflection probability \( P_r = j_r/j_i \) it is convenient to define a second measure \( \eta \) for the shielding efficiency

\[
\eta = j_r/(j_t + j_i + j_r) = j_r/(j_i - j_r),
\]

which gives the ratio of (good) reflected flux to (bad) lost flux. \( \eta \) is convenient for logarithmic plots. A reflection probability of 50% corresponds to \( \eta = 1 \). 99.9% reflection probability corresponds to \( \eta \approx 1000 \) while 0.1% reflection probability corresponds to \( \eta \approx 0.1 \).

Figure 7(a) shows the decadic logarithm of \( \eta \) (i.e. \( \log_{10}(\eta) \)) as a function of \( \Delta \) and \( \Omega \) for a collision energy of 1 mK \( \times k_B \). The solid black contours labeled by ‘0’, ‘1’ and ‘2’ correspond to a reflection probability of \( P_r = 50\% \), 91\% and 99\%, respectively. Quite generally, the shielding efficiency \( \eta \) increases with coupling strength \( \Omega \). Furthermore, for a given \( \Omega \), shielding is best for \( \Delta \approx \Omega \) (see dashed black line). If \( \Delta \) becomes too large, the repulsive barrier becomes so small, that either strong tunneling through the barrier occurs or flux even passes over the barrier. Fig. 7(b) illustrates this in a plot of the transmission probability \( P_t \). \( P_t \) increases with \( \Delta \) and decreases with \( \Omega \). We have numerically checked that the transmission probability distribution \( P_t \) shown in the Fig. 7(b) can be approximately reproduced with the well-known expression for 1D-tunneling

\[
P_t = \exp \left( -2 \frac{\sqrt{T_p}}{\hbar} \int_{T_{p1}}^{T_{p2}} \sqrt{V(r)-E_{\text{coll}}} \, dr \right),
\]

where \( T_{p1} \) and \( T_{p2} \) are the classical turning points. This means that within the shown parameter range, the transmission is dominated by tunneling but not by non-adiabatic transmission at the two classical turning points. For \( \Delta > 0 \), we find that the barrier is approximately described by a Lorentzian profile,

\[
V(r) \approx V_0 \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + (r - r_s)^2},
\]

where \( V_0 = 0.5(-\Delta + \sqrt{\Omega^2 + \Delta^2}) \hbar \) and width \( \Gamma = \sqrt{2\Omega^2 \hbar/(V_0 |k_H|)} \). Here, \( k_H \) is the curvature of the potential curve \( V_c \) at the tip. For tunneling through a Lorentzian profile analytical results can be derived, see appendix C.

Next, we will discuss non-adiabatic transitions which leak flux to the lower potential energy curve \( V_l \). Fig. 7(c) shows the probability for this leakage \( P_l \) as a function of \( \Omega \) and \( \Delta \). In the range shown, \( P_l \) decreases monotonically with increasing \( \Omega \) and \( \Delta \). While it is plausible, that a larger \( \Omega \) generally improves the adiabaticity, we note that for vanishing \( \Omega \) the leakage also will vanish because the channels \( V_c \) and \( V_g \) are not coupled anymore. Therefore, for fixed \( \Delta \) and \( E_{\text{coll}} \), \( P_l(\Omega) \) is not monotonic everywhere but must exhibit a maximum at a value below the shown range. The dependence of \( P_l \) on \( \Delta \) in Fig. 7(c), can be understood as follows. For \( \Delta < 0 \) a decrease of \( \Delta \) decreases the slope \( dV_c/dr \) at the crossing, which helps the adiabaticity according to our discussion in section II.

For \( \Delta > 0 \) there is an inherent momentum mismatch for coupling flux from the upper to the lower channel, which suppresses non-adiabaticity. The mismatch and therefore the adiabaticity increase with \( \Delta \).

From the discussion in section II where the avoided crossing with a linear potential energy curve is studied one might expect that for \( \Delta < 0 \) the leakage \( P_l \) is a Landau-Zener-like function of the scaled quantity \( -\Omega/\sqrt{2E_{\text{coll}}} \). \( \Delta = 2\pi \times 1 \) GHz. \( \log \approx \log_{10} \) is the decadic logarithm. The plots above and on the right hand side of each contour plot are cuts as indicated by the corresponding lines in the contour plots.

\[
P_l \approx \exp(c_1 + c_2 \hbar/\Omega/E_s + c_3 \hbar\Delta/E_s),
\]

where \( E_s = 0.5\hbar\sqrt{k_H/\mu} \) is an energy scale as determined by the negative curvature \( k_H = -d^2V_c/dr^2 \) of the barrier at its peak, see appendix C for details. The coefficients \( c_i \) vary slowly with \( \Omega \) and \( \Delta \). For a small enough collision energy \( E_{\text{coll}} \), \( P_l \) scales like a power law, i.e. \( P_l \propto (E_{\text{coll}}/E_s)^\alpha \). Here, \( \alpha \) is a slowly varying function of \( \hbar\Omega/E_s \) and \( \hbar\Delta/E_s \). This means that the coefficients \( c_i \) in Eq. 17 can be expanded as

\[
c_i = c_{i,1} + c_{i,2} \ln(E_{\text{coll}}/E_s).
\]

Figure 7(d) shows the shielding efficiency \( \eta \) on a logarithmic scale versus initial atomic collision energy \( E_{\text{coll}} \).

FIG. 7: (a) Shielding efficiency \( \eta \) as a function of laser detuning \( \Delta \) and coupling strength \( \Omega \) for a collision energy of 1 mK \( \times k_B \). The dashed black line indicates the best choice of \( \Delta \) to reach optimal shielding for a given \( \Omega \). (b) and (c) show the transmitted fraction \( P_t \) and the non-adiabatic leaking fraction \( P_l \) versus \( \Delta \) and \( \Omega \). (d) shows \( \eta \) versus \( \Omega \) and collision energy \( E_{\text{coll}} \). \( E_{\text{coll}} \) is in units of K \( \times k_B \). \( \Delta = 2\pi \times 1 \) GHz. \( \log \equiv \log_{10} \) is the decadic logarithm. The plots above and on the right hand side of each contour plot are cuts as indicated by the corresponding lines in the contour plots.
and $\Omega$. Here, $\Delta$ is fixed at $\Delta = 2\pi \times 1$ GHz. As expected, shielding improves as the collision energy is lowered, because both tunneling and non-adiabaticity are increasingly suppressed.

Similar as for the non-adiabatic leakage, $\eta$ exhibits approximately power law scaling, $\eta \propto (E_{coll}/E_s)^{\alpha}$, as long as the collision energies $E_{coll}$ are small enough. As before the exponent $\alpha$ depends again on $\hbar\Omega/E_s$ and $\hbar\Delta/E_s$.

### Conclusion

In conclusion, we propose a method for shielding a cold neutral atom and an ion from a collision at close range. When the particles reach an inter-particle distance on the order of 100 nm the neutral atom is resonantly excited to a low-field seeking Rydberg level which is repelled by the ion. Upon leaving the neutral atom is de-excited back in an adiabatic way, so that no spontaneous scattering of photons occurs. We find that this shielding scheme works especially well when employing an avoided crossing of two Rydberg levels. We discuss how shielding depends on the Rabi frequency of the laser, on the laser detuning of two Rydberg levels. We discuss how shielding improves as the collision energy is low.

In order to numerically integrate the Schrödinger equation it can be advantageous from a numerical point of view to locally express the two-component wavefunction $\Psi = (\varphi_U, \varphi_L)^T$ in a basis for which the interaction Hamiltonian $V_I$ is diagonal. This is done by the following transformation $S^{-1}\Psi = \Phi \equiv (\varphi_U, \varphi_L)^T$ (see [27]), where $S$ diagonalizes $V_I$ by

$$\hat{S}^{-1}V_I\hat{S} = \begin{pmatrix} V_U(r) & 0 \\ 0 & V_L(r) \end{pmatrix}.$$  \hspace{1cm} (19)

We note that $\hat{S}$ is unitary, i.e. $\hat{S}^{-1} = \hat{S}^\dagger$. This basis change transforms the Schrödinger equation into

$$\left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \hat{R} + \begin{pmatrix} V_U(r) & 0 \\ 0 & V_L(r) \end{pmatrix} \right) \Phi = E_{coll}\Phi,$$  \hspace{1cm} (20)

where $\hat{R} = \hat{R}_1 + \hat{R}_2$ is the non-adiabaticity operator with

$$\hat{R}_1 = -\frac{\hbar^2}{\mu} \hat{S}^{-1} \begin{pmatrix} d\hat{S}/dr \\ d\hat{S}/dr \end{pmatrix} \frac{d}{dr},$$  \hspace{1cm} (21)

$$\hat{R}_2 = -\frac{\hbar^2}{2\mu} \hat{S}^{-1} \begin{pmatrix} d^2\hat{S}/dr^2 \\ d^2\hat{S}/dr^2 \end{pmatrix}.$$  \hspace{1cm} (22)

Expressing $\hat{R}_1$ and $\hat{R}_2$ in terms of matrices,

$$\hat{R}_1 = \begin{pmatrix} R_{1dd} & R_{1nd} \\ -R_{1nd} & R_{1dd} \end{pmatrix} \frac{d}{dr},$$  \hspace{1cm} (23)

$$\hat{R}_2 = \begin{pmatrix} R_{2dd} & R_{2nd} \\ -R_{2nd} & R_{2dd} \end{pmatrix},$$  \hspace{1cm} (24)

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### Appendix

#### A. Numerical solution of the Schrödinger equation

Here, we describe how we determine the scattering solution of the Schrödinger equation Eq. (2) for the interaction potential of Eq. (13). We are looking for a particular solution where atom and ion with collision energy $E_{coll}$ (defined at $r = \infty$) initially approach each other in the ground state channel and the Rydberg channel is negligible. According to the boundary condition of having the incoming wave in the ground state and approaching from $r = \infty$, the wavefunction components $\varphi_U$ and $\varphi_L$ at $r_0$ must be outgoing with respect to the avoided crossing, i.e. $\propto \exp(-ik_jr)$ with the local wavenumber $k_j = \sqrt{2\mu(E_{coll} - V_j(r_0))}/\hbar$ for $j \in \{U, L\}$. This determines the derivatives of the wavefunction components at this point to be $d\varphi_j/dr = -ik_j\varphi_j$. We separately carry out two integrations with two linear independent starting vectors ($\varphi_U(r_0), \varphi_L(r_0)$)$^T$. Afterwards, the two solutions are linearly combined to provide the desired final solution $\Psi$ which fits the boundary condition.

Finding the scattering solution for the interaction potential of Eq. (1) is analogous, apart from setting $d\varphi_U/dr(r_0) = k_U\varphi_U(r_0)$ with $k_U = \sqrt{2\mu(E_U(r_0) - E_{coll})}/\hbar$. After the numerical solution of the Schrödinger equation the wavefunctions can be expressed again in the non-adiabatic basis $|g\rangle$ and $|e\rangle$ as described in appendix B.
we obtain the coupled Schrödinger equation in the following form,

\[
\frac{d^2 \varphi_U}{dr^2} = -2m \left[ (E_{coll} - V_U - R_{2d}) \varphi_U - R_{1d} \frac{d \varphi_U}{dr} \right. \\
- R_{1nd} \frac{d \varphi_L}{dr} - R_{2nd} \varphi_L], \\
\frac{d^2 \varphi_L}{dr^2} = -2m \left[ (E_{coll} - V_L - R_{2d}) \varphi_L + R_{1nd} \frac{d \varphi_U}{dr} \\
+ R_{2nd} \varphi_U - R_{1d} \frac{d \varphi_L}{dr} \right].
\]

(25)

The non-diagonal elements of \( \hat{R} \) mix the channels \( U \) and \( L \). They are only appreciable close to the avoided crossing.

C. Approximate analytic expression for the tunneling amplitude

Here, we derive an approximate, analytical expression for the tunneling probability \( P_t \) through the barrier in channel \( U \) for the case \( \Delta > 0 \). The textbook expression for the transmission probability through a barrier is

\[
P_t = \exp \left( -2\sqrt{\frac{2m}{\hbar}} \int_{T_{p1}}^{T_{p2}} \sqrt{V - E_{coll}} \, dr \right),
\]

(27)

where \( T_{p1} \) and \( T_{p2} \) are the classical turning points. As in appendix D we make the approximations that \( \Omega \) is independent of \( r \), that \( V_e = -0.5 k_H (r - r_s)^2 - \hbar \Delta \) is simply harmonic and that \( V_g = 0 \). For \( \Delta > 0 \), the adiabatic potential \( V_U \) then approximately has the shape of a Lorentzian,

\[
V_U(r) \approx V_0 \frac{(\Gamma/2)^2}{(\Gamma/2)^2 + (r - r_s)^2},
\]

(28)

with height \( V_0 = 0.5(\Delta + \sqrt{\Delta^2 + \Gamma^2}) \hbar \) which for \( \Omega \ll \Delta \) goes over into the well-known expression for the light shift, \( V_0 = \Omega^2 \hbar/(4\Delta) \).

The width of the barrier is given by \( \Gamma = \sqrt{2\Omega^2 \hbar/(V_0 k_H)} \) which for the same limit, \( \Omega \ll \Delta \), goes over into \( \Gamma = \sqrt{8\hbar \Delta k_H} \). The classical turning points are \( T_{p1} = T_{p2} = \frac{\Gamma}{2} \sqrt{1 + \frac{k_H}{\Delta}} \), using \( \beta = E_{coll}/V_0 \).

The integral of Eq. (27) can be analytically solved, yielding

\[
P_t = \exp \left( -2\sqrt{\frac{2m}{\hbar}} \frac{V_0}{\beta} \frac{\Gamma(1 - \beta)}{\hbar} C(\beta) \right),
\]

(29)

where

\[
C(\beta) = \int_{-1}^{1} \frac{1 - y^2}{\gamma y^2 + 1} \, dy \\
= -\frac{2}{\gamma} \left[ E(-\gamma) - (\gamma + 1) K(-\gamma) \right].
\]

(30)

Here, \( \gamma = (1 - \beta)/\beta \), and the functions \( K \) and \( E \) are the complete elliptic integrals for the first and second kind, respectively. \( C(\beta) \) can be approximated by the simple expression \( C(\beta) \approx 0.226 \ln(\beta) + \pi/2 \) in the relevant range 0.01 \( \leq \beta \leq 0.99 \).

D. Harmonic barrier model

We consider here the special case where the potential barrier \( V_e \) (see e.g. Fig. 4(a) and (c)) is purely harmonic and radially symmetric, i.e. \( V_e = -0.5 k_H (r - r_s)^2 - \Delta \hbar \) and the coupling \( \Omega \) between ground and excited state does not depend on \( r \). We ignore the \( 1/r^4 \) dependence of the polarization potential of the ground state and set \( V_g = 0 \). The radial Schrödinger equation for \( s \)-waves then reads

\[
-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} \Psi + \left( \frac{0}{\hbar \Omega/2} \right) \Psi = E_{coll} \Psi.
\]

(31)

Similar as for a harmonic oscillator, "Hooke’s constant" \( k_H \) introduces an energy scale \( E_s = 0.5 \hbar \sqrt{k_H/\mu} \), and a length scale \( l_s = \hbar \sqrt{1/(2\mu E_s)} \). In units of these two scales the Schrödinger equation becomes

\[
-\frac{d^2}{dr^2} \Psi + \left( \frac{0}{\Omega/2} \right) \Psi = \tilde{E}_{coll} \Psi.
\]

(32)

where \( \tilde{r} = (r - r_s)/l_s \), \( \tilde{\Omega} = \hbar \Omega/E_s \), \( \tilde{\Delta} = \hbar \Delta/E_s \), and \( \tilde{E}_{coll} = E_{coll}/E_s \). Thus, the solution of the problem, along with the transmission, reflectivity, and the non-adiabaticity of the effective barrier, only depends on the three dimensionless parameters \( \Omega, \tilde{\Delta}, \tilde{E}_{coll} \).

E. Rabi frequency \( \Omega \) for arbitrary collision angles

Here, we calculate the Rabi frequency \( \Omega \) (along with the effective transition dipole matrix element \( \delta_{d1} \)) for an optical transition from the atomic ground state to a Rydberg state for the case when the quantization axis \( z \) is not collinear with the internuclear axis \( z' \) of atom and ion. Let the ground state atom be in the state \( |g\rangle = \sum_m \beta_m |j,m\rangle \). Let the electrical component of the coherent light field be \( \vec{E} \equiv (E_x, E_y, E_z) \). The light field can be decomposed into the spherical components:

\[
E_1 = -\frac{1}{\sqrt{2}} (E_x + iE_y) = \mathcal{E} a_1, \\
E_0 = E_z = \mathcal{E} a_0, \\
E_{-1} = \frac{1}{\sqrt{2}} (E_x - iE_y) = \mathcal{E} a_{-1},
\]

(33)

(34)

(35)

where \( \mathcal{E} = \sqrt{E_x^2 + E_y^2 + E_z^2} \) and the \( \{a_i\} \) are relative amplitudes of the light polarization components. Let \( \theta \) be the angle between the quantization axis \( z \) and the internuclear axis \( z' \). \( \theta \) is corresponding rotation vector which
is perpendicular to both the quantization axis $z$ and the internuclear axis $z'$ and has length $\theta$. We can generate a \{\{x', y', z'\}\} coordinate system by rotating the \{\{x, y, z\}\} coordinate system by $\vec{\theta}$. Viewed in the \{\{x', y', z'\}\}-frame the atomic ground state reads

$$|g\rangle' = \sum_{m, \tilde{m}} R^1_{\tilde{m}, m}(-\vec{\theta}) \beta_m |j, \tilde{m}\rangle,$$

where $R^1_{\tilde{m}, m}(-\vec{\theta}) = \langle j, \tilde{m} | R(-\vec{\theta}) | j, m \rangle$ are the matrix elements of the rotation operator $R(-\vec{\theta}) = \exp(-i\vec{\theta} \cdot \vec{j})$. Here, $\vec{j}$ is the angular momentum operator. The polarization \{\{a_i\}\} of the light in the \{\{x, y, z\}\}-frame, transforms into \{\{a'_i\}\} for the rotated \{\{x', y', z'\}\}-frame, where $a'_i = \sum_k R^1_{k, i}(-\vec{\theta}) a_i$.

The atom-light interaction Hamiltonian is given by

$$H_{AL} = e \vec{r}_e \cdot \vec{E} = e \sum_i r_{e, i} E_i = e \mathcal{E} \sum_i r_{e, i} a_i,$$

where

$$r_{e, 1} = -\frac{1}{\sqrt{2}} (x_e + iy_e),$$

$$r_{e, 0} = z_e,$$

$$r_{e, -1} = \frac{1}{\sqrt{2}} (x_e - iy_e),$$

are the spherical components of $\vec{r}_e$. The components $r_{e, 1}, r_{e, 0}, r_{e, -1}$ can be viewed as operators which induce $\sigma^+, \pi, \sigma^-$ transitions, respectively, so that the $m$-quantum number of the atom changes by $1, 0, -1$, respectively.

In the rotated coordinate system \{\{x', y', z'\}\} the Hamiltonian for atom-light interaction reads

$$H_{AL} = e \mathcal{E} \sum_i r'_{e, i} a'_i,$$

$$= e \mathcal{E} \sum_{i, k} r'_{e, i} R^1_{i, k}(-\vec{\theta}) a_k,$$

Therefore, the transition matrix element to the Rydberg state $|e, m'\rangle$ is given by

$$\langle e, m'| H_{AL} | g \rangle' = \mathcal{E} \langle e, m'| \sum_{i, k} e r'_{e, i} R^1_{i, k}(-\vec{\theta}) a_k | g \rangle'$$

$$= \mathcal{E} \sum_{i, m, k} \langle e, m'| e r'_{e, i} | j, \tilde{m}\rangle R^1_{i, k} a_k R^2_{\tilde{m}, m} \beta_m,$$

where in the last line we have omitted the argument $(-\vec{\theta})$ in the rotation matrix elements. The term $\langle e, m'| e r'_{e, i} | j, \tilde{m}\rangle = d_{el,i} (m', \tilde{m})$ is the electric dipole transition matrix element, as defined and calculated earlier in the main text. Apart from a constant factor, the transition matrix element equals the Rabi frequency $\Omega_{m'}$,

$$\langle e, m'| H_{AL} | g \rangle \equiv \hbar \Omega_{m'}/2.$$

Besides $|e, m'\rangle$ also the Rydberg state $|e, -m'\rangle$ might be resonantly addressed by the coherent optical light field, since the two Rydberg states are energetically degenerate. In fact, the optical light field \{\{a_i\}\} drives a transition from the ground state $|g\rangle$ towards the state $|e_c\rangle$ within the degenerate Rydberg manifold spanned by $|e, \pm m'\rangle$. The Rabi frequency for this transition to $|e_c\rangle$ is $\Omega = \sqrt{\Omega^2_{m'} + \Omega^2_{-m'}}$. The effective transition dipole moment for the transition to the state $|e_c\rangle$ is $d_{el}(e_c, g, \{a_i\}, \vec{\theta}) = \hbar \Omega/(2 \mathcal{E})$.

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[28] This procedure ignores the fact that the electric field of the ion is inhomogeneous. An approach where the inhomogeneity is correctly taken into account is given in section IIIB.
[29] The quantum defect for the \(nP_{3/2}\) state of \(^{87}\)Rb is given by \(\delta(n) = \delta_0 + \delta_2/(n-\delta_0)^2\), where \(\delta_0 = 2.6416737(10)\) and \(\delta_2 = 0.2950(7)\) [23].
[30] Due to hyperfine interaction, the quantum state of ground state \(^{87}\)Rb is normally described in terms of the quantum numbers \(f, m_f\) corresponding to the total angular momentum \(\vec{f} = \vec{j} + \vec{i}\) with nuclear spin \(i\). Pure \(m_j = \pm 1/2\) states can be prepared by working with the spin stretched states \(|f = 2; m_f = \pm 2\rangle\).