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Trapped Ions in Rydberg-Dressed Atomic Gases

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We theoretically study trapped ions that are immersed in an ultracold gas of Rydberg-dressed atoms. By off-resonant coupling on a dipole-forbidden transition, the adiabatic atom-ion potential can be made repulsive. We study the energy exchange between the atoms and a single trapped ion and find that Langevin collisions are inhibited in the ultracold regime for these repulsive interactions. Therefore, the proposed system avoids recently observed ion heating in hybrid atom-ion systems caused by coupling to the ion's radio frequency trapping field and retains ultracold temperatures even in the presence of excess micromotion.

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Introduction.—Recent years have seen significant interest in coupling ultracold atomic and ionic systems [1–5] with the purpose of realizing quantum simulators [6,7], studying ultracold chemistry [8,9] and collisions, or employing ultracold gases to sympathetically cool trapped ions [10–12]. It has become clear, however, that the time-dependent trapping field of Paul traps limits attainable temperatures in interacting atom-ion systems [2,3,11–17]. This effect stems from the fast micromotion of ions trapped in radio frequency traps, which may add significant energy to the system when short-range (Langevin) collisions with atoms occur.

Here, we theoretically study ionic impurities immersed in a cloud of atoms that are coupled to Rydberg states [18–23]. By selecting a Rydberg state that is coupled to the ground state via a dipole-forbidden transition, we can change the atom-ion interaction such that it becomes repulsive for ultracold atoms. In this situation, the atoms cannot get close enough to the ion for the trap drive to add energy to the system, and no excess heating takes place. Instead, the system slowly thermalizes at a rate that is compatible to the rate expected for an ion trapped in a time-independent trap. We also show that in contrast to ground-state (attractive) atom-ion systems, which require the mass of the ion to be larger than that of the atom [14–17,24–26], the proposed scheme retains ultracold temperatures for the combinations ^{87}Rb - $^{171}\text{Yb}^+$ and ^{87}Rb - $^9\text{Be}^+$ alike.

The Letter is organized as follows. First, we will describe how the atom-ion interaction can be engineered to be repulsive by coupling to a Rydberg state. Second, we will show that such an atom-ion potential does not lead to heating when the ion is trapped in a Paul trap and is interacting with a cloud of atoms. For this, we will use a classical description of the atom-ion dynamics [12,14]. Finally, we discuss possible experimental issues and limitations of our proposed system.

Dressing on a dipole-forbidden transition.—We are interested in dressing an alkali atom in the ground state

$|gS\rangle$ with a Rydberg state $|nS\rangle$ using a single near-resonant laser field, as shown in Fig. 1. When there are no electric fields present, such a transition is prohibited. However, the field of a nearby ion may mix $|nS\rangle$ with Rydberg states that can couple to the $|gS\rangle$ state via a laser field. Within the dipole approximation and using perturbation theory we obtain the following for the Rydberg wave function:

$$|\psi(\mathbf{R})\rangle \approx |nS\rangle + eE_{\text{ion}}(\mathbf{R}) \sum_k \frac{\langle kP|z|nS\rangle}{\mathcal{E}_{nS} - \mathcal{E}_{kP}} |kP\rangle, \quad (1)$$

where $\mathcal{E}_j$ denotes the energy of state $|j\rangle$ and $E_{\text{ion}}(\mathbf{R})$, with $\mathbf{R} = \mathbf{r}_i - \mathbf{r}_a$, denotes the electric field generated by an ion located at position $\mathbf{r}_i$, evaluated at the atomic position $\mathbf{r}_a$. The relative electron-atom core position projected on the electric field direction is denoted by z , where we assume a reference frame in which the local electric field $\mathbf{E}_{\text{ion}}(\mathbf{R})$ always points in the z direction. In this picture, only states with magnetic quantum number $m_L = 0$ are mixed into $|\psi(\mathbf{R})\rangle$ by the field. For further simplification we have neglected fine-structure effects for now; this is justified when the laser detuning is much larger than the fine-structure splitting of the $|kP\rangle$ Rydberg levels, which will usually be the case. Using expression (1) for the Rydberg state, we can estimate the Rabi frequency for one-photon coupling to the ground state $\Omega(\mathbf{R}) = e\langle\psi(\mathbf{R})|\mathbf{E}_L \cdot \mathbf{r}|gS\rangle/\hbar$, where $\mathbf{E}_L$ denotes the electric field of the laser within the rotating wave approximation and $\mathbf{r}$ the position of the electron in the lab frame. Combining this equation with Eq. (1), we get

$$\Omega(\mathbf{R}) \approx \frac{e^2 \mathbf{E}_L \cdot \mathbf{E}_{\text{ion}}(\mathbf{R})}{\hbar} \sum_k \frac{\langle nS|z|kP\rangle}{\mathcal{E}_{nS} - \mathcal{E}_{kP}} \langle kP|z|gS\rangle. \quad (2)$$

Now we can see what happens if we dress the ground state $|gS\rangle$ with $|\psi(\mathbf{R})\rangle$. For large distances $R \rightarrow \infty$, the transition between $|gS\rangle$ and $|\psi(\mathbf{R})\rangle$ will be dipole forbidden and no dressing occurs. As the distance decreases, the $|nS\rangle$ state gets

polarized by the ion and its adiabatic energy shift is given to lowest order by $V_{nS}(R) = -C_4^{nS}/R^4$ [27]. We can find the dressed potential by looking at the two-level Hamiltonian in the $|gS\rangle, |\psi(\mathbf{R})\rangle$ subspace after performing the rotating wave approximation,

$$H_{2\text{-level}} = \begin{pmatrix} -\frac{C_4^{gS}}{R^4} & \hbar\Omega(\mathbf{R}) \\ \hbar\Omega^*(\mathbf{R}) & -\hbar\Delta_0 - \frac{C_4^{nS}}{R^4} \end{pmatrix}, \quad (3)$$

where we for now neglected any off-resonant couplings and assumed that the laser is blue-detuned by Δ_0 from the $|gS\rangle \rightarrow |nS\rangle$ transition and that this detuning is much smaller than the level splitting between $|nS\rangle$ and all other Rydberg states. In the dispersive limit, where $\hbar|\Omega(\mathbf{R})| \ll \hbar\Delta_0 + C_4^{nS}/R^4$ and $C_4^{gS} \ll C_4^{nS}$, diagonalization results in the following dressed potential:

$$V_d(\mathbf{R}) \approx \frac{\hbar^2|\Omega(\mathbf{R})|^2}{\hbar\Delta_0 + C_4^{nS}/R^4} - \frac{C_4^{gS}}{R^4}. \quad (4)$$

In order to proceed, we need to evaluate $|\Omega(\mathbf{R})|^2$, which now depends on the atom-ion separation. We have $|\Omega(\mathbf{R})|^2 = |\beta(\theta, \phi)|^2/R^4$, with

$$\beta(\theta, \phi) = \frac{e^3 E_L^\parallel(\theta, \phi)}{4\pi\epsilon_0 \hbar} \sum_k \frac{\langle nS|z|kP\rangle \langle kP|z|gS\rangle}{\mathcal{E}_{nS} - \mathcal{E}_{kP}}. \quad (5)$$

Here, $E_L^\parallel(\theta, \phi) = \mathbf{E}_L \cdot \mathbf{E}_{\text{ion}}(\mathbf{R})/|\mathbf{E}_{\text{ion}}(\mathbf{R})|$ denotes the projection of the laser's electric field onto the electric field of the ion, and θ and ϕ denote the azimuthal and polar angle of $\mathbf{R}$ according to the laboratory reference frame, respectively. Combining Eqs. (4) and (5), our final result within first-order perturbation theory is

$$V_d(\mathbf{R}) = \frac{A(\theta, \phi)R_w^4}{R^4 + R_w^4} - \frac{C_4^{gS}}{R^4}. \quad (6)$$

The first term in the potential (6) is repulsive and has a maximum height $A(\theta, \phi) = \hbar^2|\beta(\theta, \phi)|^2/C_4^{nS}$ and width $R_w = [C_4^{nS}/(\hbar\Delta_0)]^{1/4}$. The angular dependence of $\beta(\theta, \phi)$ is determined by the laser polarization. For linear polarization along the z direction of the laboratory frame, for instance, we have $\mathbf{E}_L^z = (0, 0, E_L)$ such that $E_L^\parallel \propto \cos\theta$, whereas circular polarization, $\mathbf{E}_L^+ = E_L(1, i, 0)/\sqrt{2}$, gives us $E_L^\parallel \propto i \sin\theta \cos\phi + \sin\theta \sin\phi$. The latter results in a donut-shaped repulsive potential in the x, y plane and no interaction along the z direction. In order to make the potential repulsive in all directions we may use two laser fields coupling on the transitions $|gS\rangle \rightarrow |nS\rangle$ and $|gS\rangle \rightarrow |n'S\rangle$, such that $R_w = R'_w = (C_4^{n'S}/\hbar\Delta_0')^{1/4}$ with Δ_0' the bare detuning on the $|gS\rangle \rightarrow |n'S\rangle$ transition. Employing the laser fields E_L^z and E_L^+ and appropriate tuning of the laser powers, such that the

FIG. 1. A trapped ion (blue sphere) in a cloud of atoms (orange spheres); the atomic ground states $|gS\rangle$ are dressed with the Rydberg state $|nS\rangle$ with n the principal quantum number and Δ_0 the laser detuning. By appropriate engineering of the Rydberg laser field, the adiabatic atom-ion potential can be made repulsive such that the atoms cannot get close enough to undergo Langevin collisions (as depicted by the sphere around the ion). To optically shield the ion in three dimensions, two laser fields are needed with linear and circular polarization, as explained in the text.

Rabi frequencies are equal, results in a spherically symmetric potential $A(\theta, \phi) = A$, as described in more detail in the Supplemental Material [28].

An example of a dressed potential calculated within first-order perturbation theory is shown in Fig. 2, where we used the approximate analytic wave functions of Ref. [31] to evaluate the matrix elements in Eq. (5) and $\Delta_0 = 2\pi \times 1$ GHz such that $R_w = 270$ nm. We also show the potential obtained by diagonalization of the Rydberg manifold in the presence of the ion electric field and dressing laser, within the rotating wave approximation, taking spin-orbit coupling and terms up to charge-quadrupole coupling into account. For these calculations, we used the quantum defects found in Ref. [30] while the Rydberg wave functions were obtained by the Numerov method [28]. This more accurate calculation shows good agreement with our approximated potential for atom-ion separations, down to about 160 nm. At close atom-ion proximity, the $|19S\rangle$ state gets strongly coupled to other Rydberg states, causing avoided crossings. However, for atom temperatures that are much smaller than the repulsive barrier, $T_a \ll A/k_B$, short-range collisions between the atoms and ion are suppressed. If we assume a Rabi frequency of $\Omega_{19P, m_L=0} = 2\pi \times 200$ MHz on the $|5S\rangle \rightarrow |19P\rangle$ transition in Rb and use that the transition-matrix elements scale as $\langle kP|r|gS\rangle \propto k^{-3/2}$, we can estimate $A/k_B \sim 27$ μ K,

which is larger than typical ultracold atom temperatures. We can therefore neglect the inner part of the dressed potential and the second term in Eq. (6) for these parameters in the ultracold regime, and for the remaining simulations in this work we replace $V_d(\mathbf{R})$ by the spherically symmetric $\tilde{V}_d(R) = AR_w^4/(R^4 + R_w^4)$.

Thermalization in Paul traps.—To investigate whether the dressed repulsive potential prevents ion heating out of the ultracold regime, we have studied classical collisions

FIG. 2. The dressed potential $V_d(R)$ assuming coupling to the $|19S\rangle$ state of Rb with $\Delta_0 = 2\pi \times 1.0$ GHz. The dashed line is calculated from the Rydberg wave functions taken from Ref. [31] in first-order perturbation theory, within the dipole approximation, and neglecting spin-orbit coupling. Here, we assumed the defects of the $L - 1/2$ for the L states and set the Rabi frequency on the $|5S\rangle \rightarrow |19P\rangle$ transition to $\Omega_{19P,m_L=0} = 2\pi \times 200$ MHz by tuning the laser intensity. The black dots are computed by diagonalization of the Rydberg manifold in the presence of the dressing laser and ion, in the rotating wave approximation, including spin-orbit coupling, up to charge-quadrupole order in the atom-ion interaction terms. The laser intensity was set to the same value as for the approximated potential. For both calculations, we took the Rydberg states $n = 10, \dots, 30$ into account [28].

between an ion and atoms. We assume that we have an ion trapped in a Paul trap generated by the electric fields $\mathbf{E}_{\text{PT}}(\mathbf{r}, t) = \mathbf{E}_s(\mathbf{r}) + \mathbf{E}_{\text{rf}}(\mathbf{r}, t)$ with

$$\mathbf{E}_s(x, y, z) = \frac{m_i \omega_z^2}{e} \left(\alpha_x \frac{x}{2}, \alpha_y \frac{y}{2}, -z \right),$$

$$\mathbf{E}_{\text{rf}}(x, y, z, t) = \frac{m_i \Omega_{\text{rf}}^2 q}{2e} \cos(\Omega_{\text{rf}} t) (x, -y, 0). \quad (7)$$

Here, Ω_{rf} is the trap drive frequency and q is the dynamic stability parameter for an ion of mass m_i and charge e . The motion of the ion in the transverse x, y direction is given by a slow secular motion of frequency $\omega_{x,y} \approx (\Omega_{\text{rf}}/2) \sqrt{a_s + q^2/2}$, with $a_s = -\alpha_{x,y} 2\omega_z^2 / \Omega_{\text{rf}}^2$ the static stability parameter, and a fast micromotion of frequency Ω_{rf} . The unitless parameters $\alpha_x + \alpha_y = 2$ are introduced to lift the degeneracy in the transverse confinement. The ion dynamics in the z direction is purely harmonic with trap frequency ω_z .

To begin with, we assume that the ion has initially no energy and sits at the center of the Paul trap as in Refs. [12,14]. The idea behind this approach is that although each individual system may be prepared in the ultracold regime by, e.g., laser and evaporative cooling, it is only when the atoms and ions are brought together that excessive heating is observed [12]. In order to simulate the

effect of the atomic cloud we calculate classical trajectories of Rb atoms, with the atoms appearing one by one on a sphere of radius $2 \mu\text{m}$ around the ion and with a velocity that is randomly picked from a Maxwell-Boltzmann distribution of temperature T_a . As soon as the atom has left the sphere around the ion at the end of the collision, we introduce a new atom to interact with the ion. We assume the atomic bath to be very large such that its temperature does not change as more collisions occur. After each collision, we obtain the ion's secular energy by fitting an approximate analytic solution of the equations of ion motion to the numerically obtained orbit (see Supplemental Material [28] and Ref. [12]). We define the ion temperature to be $T_{\text{ion}} = \bar{\mathcal{E}}/(3k_B)$ with $\bar{\mathcal{E}}$ the total average secular energy of the ion. Assuming $^{171}\text{Yb}^+$ for the ion, we set $\Omega_{\text{rf}} = 2\pi \times 2$ MHz and $\omega_x = 2\pi \times 54$ kHz, $\omega_y = 2\pi \times 51$ kHz, and $\omega_z = 2\pi \times 42$ kHz.

We first study the case where the atoms are not dressed to a Rydberg state. Thus, we set the atom-ion interaction to $V_{ai}(R) = -C_4^{gs}/R^4 + C_6/R^6$, where the first term denotes the ground-state atom-ion-induced polarization-charge interaction and the second term accounts for some short-range repulsion, which we set to dominate for $R < 10$ nm. The results of averaging 100 of these simulation runs can be seen in the inset of Fig. 3. From the individual trajectories, it is clear that most atoms fly by the ion without causing much effect. One in a few hundred collisions, however, is of the Langevin type, causing significant energy exchange. The ion quickly heats up to temperatures much higher than the atomic cloud temperature of $2 \mu\text{K}$. These observations are in line with the findings of Refs. [12,14]. If we simulate more collisions, finite-size effects start to limit the accuracy of these calculations, as the ionic oscillation amplitude becomes comparable to the radius of the sphere of atomic starting positions. For comparison, we also show the results obtained when assuming that the ion is in a time-independent trap with the same trap frequencies (the secular approximation). Here, we see that the ion slowly thermalizes with the atomic gas.

Now, we will study how these dynamics change for the Rydberg-dressed atoms for which the atom-ion interaction is repulsive. We replace $V_{ai}(R)$ by $\tilde{V}_d(R)$ with $A/k_B = 27 \mu\text{K}$ and $R_w = 270$ nm, leaving all other parameters in the simulation the same. The results can be seen in Fig. 3: the ion thermalizes slowly with the atomic cloud after about $4 \times 10^3 (1/e)$ collisions. Starting with an initial ion velocity of $0.02(1, 1, 1)$ m/s, which corresponds to an initial energy of $\sim 4 \mu\text{K}$, we can also simulate cooling of the ion towards the temperature of the atomic gas. Up until now, we have assumed ideal experimental conditions in which the minima of $\mathbf{E}_s(\mathbf{r})$ and $\mathbf{E}_{\text{rf}}(\mathbf{r}, t)$ are perfectly overlapped. In practice however, stray electric fields may cause the trap center to not coincide with the radio frequency null. This causes additional ion motion known as excess micromotion [32]. To study its effect, we introduce an additional electric

FIG. 3. Collision dynamics for an $^{171}\text{Yb}^+$ ion in a Rydberg-dressed Rb gas with repulsive interactions and $T_a = 2 \mu\text{K}$. The ion heats up from $T_{\text{ion}} = 0$ to about $1.8 \mu\text{K}$, corresponding to near thermalization. Excess micromotion due to a dc field of $E_{\text{EMM}} = 0.05$ V/m does not affect the thermalization dynamics, which is completely equivalent to that expected for an ion trapped in a time-independent trap with the same secular trap frequencies. For the curve starting at around $4 \mu\text{K}$, we gave the ion an initial velocity of $0.02(1,1,1)$ m/s and we simulate cooling towards the atomic gas temperature. The fastest thermalization curve shows the results for the combination $^{87}\text{Rb}/^9\text{Be}^+$. The inset shows results for ground-state atoms, in which the interaction is attractive. Even without excess micromotion, the ion quickly heats up to temperatures higher than the atomic cloud, whereas within the secular approximation slow thermalization would occur. All results represent the average of 50–100 runs.

field of $\mathbf{E}_{\text{EMM}} = (0.05, 0, 0)$ V/m, which displaces the potential minimum by $x_{\text{EMM}} = 243$ nm, corresponding to an average kinetic energy of $\mathcal{E}_{\text{EMM}}/k_B = m_i q^2 \Omega^2 x_{\text{EMM}}^2 / (16k_B) \approx 100 \mu\text{K}$, and run the simulations. For the repulsive case we find that the dynamics are not affected by the excess micromotion, confirming that the repulsive potential prevents excessive heating of the ion in the Paul trap. Indeed, we repeated the simulation assuming a time-independent potential with the same secular trap frequencies and see no differences beyond statistical fluctuations due to the random atom sampling. Hence, the repulsive potential allows us to make the secular approximation in the hybrid atom-ion system for the parameters used. Note that the assumption that the atom and ion cannot undergo short-range collisions still holds in this case as long as the amplitude of oscillation $r_{\text{EMM}} = qx_{\text{EMM}}/2 \sim 10$ nm $\ll R_w$, even though $\mathcal{E}_{\text{EMM}}/k_B > A/k_B$.

Finally, we study the effect of the atom-ion mass ratio for the repulsive case. For attractive atom-ion interactions it is well known that stable cold trapping can only be achieved as long as $m_a \lesssim m_i$, with m_a the mass of the atom [14–17, 24–26]. To see how this changes for the repulsive case, we repeated the simulations for the combination $^{87}\text{Rb}/^9\text{Be}^+$, whose mass ratio lies far outside of the range where

thermalization can be expected. As can be seen in Fig. 3, this combination also remains within the ultracold regime when the interactions are repulsive, thermalizing after about 2×10^3 ($1/e$) collisions.

Experimental issues.—For the calculations in this Letter we have neglected the effect of the ionic trapping fields on the dressing of the atom. This is justified since the trapping field at maximal amplitude is much smaller than the field of the ion at the dressing point: $\max[E_{\text{PT}}(R_w, t)]/E_{\text{ion}}(R_w) \approx 10^{-4}$ ($\approx 10^{-5}$ for $^9\text{Be}^+$), such that we can safely neglect these fields. Far away from the center of the trap, however, the maximal amplitude of the trapping fields becomes similar to $E_{\text{ion}}(R_w)$. For the numbers used in this Letter, this occurs only at $R \approx 1$ mm from the trap center, such that we can also safely neglect the effect of the dressing on the atomic cloud far away from the ion.

For the simulations, we assumed that only a single atom was interacting with the ion at the same time, which would require a density of $\rho_a \leq 1/R_w^3 \approx 10^{19} \text{ m}^{-3}$. Assuming an atomic density of $\rho_a = 10^{18} \text{ m}^{-3}$ and $T_a = 2 \mu\text{K}$, we have a flux of about 6×10^5 atoms/s entering the sphere of $R = 2 \mu\text{m}$, such that each collision in Fig. 3 amounts to a few μs . We estimate an upper bound to the photon scattering rate as $\Gamma \leq f\Gamma_{195}\rho_a R_w^3 \approx 10$ Hz, for $\rho_a = 10^{18} \text{ m}^{-3}$, with Γ_{195} the decay rate of the Rydberg state and f the probability for an atom to be found in the Rydberg state, $f \propto \hbar^2 |\Omega(\mathbf{R})|^2 / (\hbar\Delta_0 + C_4^s/R^4)^2 \leq 10^{-3}$. Therefore, we expect that photon scattering will not considerably affect the collision dynamics. For increasing ion temperatures, there is a probability that the atom makes it over the repulsive barrier in a collision. To investigate this regime, we simulated 2×10^5 collisions between atoms with $T_a = 2 \mu\text{K}$ and T_{ion} about $100 \mu\text{K}$; we found that in 146 instances, the atoms approached the ion to distances below $R_w/2$, such that they entered the inner regime of the dressed potential. For T_{ion} around $10.6 \mu\text{K}$, the number of atoms entering the inner part of the potential dropped to zero [28]. We conclude that our scheme works best for ions and atoms that are precooled into the ultracold regime before the systems are merged. Finally, we estimate the probability P_{tunnel} for the atom to tunnel through the potential barrier to be $P_{\text{tunnel}} \approx \exp(-\sqrt{2\mu_{ai}}(A - k_B T_a)/\hbar^2 R_w) \sim 10^{-9}$, with μ_{ai} the atom-ion reduced mass, such that we can safely neglect this effect.

Conclusions.—We have shown that trapped ions in Rydberg-dressed gases are stable against micromotion-assisted heating when we design the dressed atom-ion potential to be repulsive. To engineer this repulsive interaction, a scheme that employs one-photon dressing on a dipole-forbidden transition can be used. While Rydberg states with negative polarizability could also be used to engineer repulsive atom-ion interactions, these are not always available or can be hard to spectrally resolve. The scheme may be employed for a wider range of atom-ion mass ratios than is the case for the attractive

atom-ion system. The results may be of interest when studying atom-ion interactions in the quantum regime and may find applications in hybrid quantum computation or simulation approaches [6,27,33] and the study of polarons [34] in these systems.

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