Trapped Ions in Rydberg-Dressed Atomic Gases

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Supplementary Material to: Trapped Ions in Rydberg-Dressed Atomic Gases

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I. SPHERICALLY SYMMETRIC POTENTIAL

We can use two dressing lasers to engineer a spherically symmetric potential, coupling on the transitions $|gS\rangle \to |nS\rangle$ and $|gS\rangle \to |n'S\rangle$. After performing the rotating wave approximation, we can write the Hamiltonian in the $|gS\rangle$, $|\psi(\mathbf{R})\rangle$, $|\psi'(\mathbf{R})\rangle$ subspace

$$H_{3-\text{level}} = \begin{pmatrix} -\frac{C_4^{gS}}{R^4} & \hbar\Omega(\mathbf{R}) & \hbar\Omega'(\mathbf{R}) \\ \hbar\Omega^*(\mathbf{R}) & -\hbar\Delta_0 - \frac{C_4^{nS}}{R^4} & 0 \\ \hbar\Omega'^*(\mathbf{R}) & 0 & -\hbar\Delta_0' - \frac{C_4^{n'S}}{R^4} \end{pmatrix}. \tag{1}$$

To obtain the adiabatic potential, we diagonalize $H_{3-\text{level}}$ assuming $\hbar|\Omega(\mathbf{R})| \ll \hbar\Delta_0 + C_4^{nS}/R^4$, $C_4^{gS} \ll C_4^{nS}$ and $\hbar|\Omega'(\mathbf{R})| \ll \hbar\Delta_0' + C_4^{n'S}/R^4$, $C_4^{gS} \ll C_4^{n'S}$ so that we can expand to second order in $\hbar|\Omega(\mathbf{R})|$ and $\hbar|\Omega'(\mathbf{R})|$ to find:

$$V_{3d}(\mathbf{R}) \approx \frac{A(\theta,\phi)R_{\text{w}}^4}{R^4 + R_{\text{w}}^4} + \frac{A'(\theta,\phi)R_{\text{w}}'^4}{R^4 + R_{\text{w}}'^4} - \frac{C_4^{gS}}{R^4}. \tag{2}$$

with $A(\theta,\phi) = \frac{\hbar^2|\beta(\theta,\phi)|^2}{C_4^{nS}}$ and $A'(\theta,\phi) = \frac{\hbar^2|\beta'(\theta,\phi)|^2}{C_4^{n'S}}$. The angular dependence of β is expressed as:

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

$$\beta'(\theta,\phi) = \frac{e^3 E_{\text{L}}'^{\parallel}(\theta,\phi)}{4\pi\epsilon_0\hbar} \sum_k \frac{\langle n'S|z|kP\rangle\langle kP|z|gS\rangle}{\mathcal{E}_{n'S} - \mathcal{E}_{kP}}. \tag{4}$$

Where $E_{\text{L}}^{\parallel}(\theta,\phi)$ denotes the projection of the laser electric field onto the electric field of the ion. Now we set $\mathbf{E}_{\text{L}} = (0, 0, E_{\text{L}})$ such that $\beta(\theta,\phi) = \beta_0\cos\theta$ and $\mathbf{E}_L' = E'_L(1, i, 0)/\sqrt{2}$ such that $\beta'(\theta,\phi) = \beta_0'(i\sin\theta\cos\phi + \sin\theta\sin\phi)$. In this situation,

$$V_{3\text{d}}(\mathbf{R}) \approx \frac{|\beta_0|^2\cos^2\theta R_{\text{w}}^4}{C_4^{nS}(R^4 + R_{\text{w}}^4)} + \frac{|\beta_0'|^2\sin^2\theta R_{\text{w}}'^4}{C_4^{n'S}(R^4 + R_{\text{w}}'^4)} - \frac{C_4^{gS}}{R^4}, \tag{5}$$

which results in a spherically symmetric potential if we set $R_{\text{w}} = R'_{\text{w}}$ and $|\beta_0|^2/C_4^{nS} = |\beta_0'|^2/C_4^{n'S}$, which can be done by tuning Δ_0, Δ_0' and the laser intensities.

II. DETERMINATION OF ION TEMPERATURE

The explicit time dependence of the electric trapping field obstructs a straight-forward definition of some physical quantities such as energy and temperature. Nonetheless, if the time dependence of the external field is periodic and the underlying equations of motion are linear, we are able to apply Floquet's theory and the problem can be decomposed into a part which oscillates with the same period as the external field and a part, referred to as the secular part, which is time independent [1]. Often useful physical quantities can be constructed from the secular problem

and its solution, e.g. in systems of multiple ions energy and temperature can be defined via the secular solutions of the linearized problem. For the combined system of atoms and ions we do not have a closed form for the solution at hand, but in the considered case of low densities the system will evolve as the uncoupled one for time periods in which all atoms are spatially well separated from the ion. During those time periods the interaction forces can be neglected and a measurement of the secular energy of the isolated ion system is possible. The ion's secular energy $\mathcal{E}$ can be determined via its secular frequencies ω_i, $i = x, y, z$, and the amplitude of the orbit's secular component. For a single ion in an oscillating electric field $\mathbf{E}_{\mathrm{PT}}(\mathbf{r}, t)$, as defined in the main text, with appropriately chosen trap parameters the equations of motion can be solved analytically and the solutions take the following approximate form

$$x(t) \approx (C_x \cos(\omega_x t) + S_x \sin(\omega_x t)) \left(1 + \frac{q}{2} \cos(\Omega_{\mathrm{rf}} t)\right) - \frac{\omega_x q}{\Omega_{\mathrm{rf}}} (S_x \cos(\omega_x t) - C_x \sin(\omega_x t)) \sin(\Omega_{\mathrm{rf}} t), \tag{6}$$

$$y(t) \approx (C_y \cos(\omega_y t) + S_y \sin(\omega_y t)) \left(1 - \frac{q}{2} \cos(\Omega_{\mathrm{rf}} t)\right) + \frac{\omega_y q}{\Omega_{\mathrm{rf}}} (S_y \cos(\omega_y t) - C_y \sin(\omega_y t)) \sin(\Omega_{\mathrm{rf}} t), \tag{7}$$

$$z(t) = (C_z \cos(\omega_z t) + S_z \sin(\omega_z t)) . \tag{8}$$

Here we neglected correction terms which oscillate faster than the trap drive frequency Ω_{rf}. Given the ion's position at two instances of time the above system of linear equations can be inverted to obtain the coefficients C_i and S_i of the secular solution's cosine and sine part. As a preliminary step the secular frequencies can be determined numerically by fitting the above analytic approximation to a numerically obtained solution. This increases accuracy as compared to the approximate analytical expression for the ω_i we gave in the main text. Given all this we can now calculate the secular energy $\mathcal{E} = \sum_{i=x,y,z} m_i \omega_i^2 (C_i^2 + S_i^2)/2$ of the isolated ion system.

In the case of the repulsive potential, which we analyzed in the main text, the strong similarity of the thermaliztion process for the full and the secular problem indicates that the ion's secular temperature for this type of potentials is indeed a meaningful physical observable, in contrast to the attractive case.

III. OVER BARRIER COLLISIONS

In our simulations of the classical collision dynamics there is a non-vanishing probability for the atoms to overcome the repulsive barrier. Since the ion is strongly localized, we estimate this to occur when the amplitude of ion oscillation exceeds R_{w}, or $T_{\mathrm{ion}} \gtrsim m_i \bar{\omega}^2 R_{\mathrm{w}}^2/(2k_{\mathrm{B}}) \approx 70 \, \mu\mathrm{K}$ for the parameters used in this work, with $\bar{\omega}$ the average trap frequency. To estimate if those events pose a problem we performed collision simulations where we kept record of the minimal separation $d_{\min}$ between atom and ion. More precisely we simulated the interaction of an ion with a bath of $T_a = 2 \, \mu\mathrm{K}$ atoms for 200 collisions. The result of 1000 such simulations for ion temperatures T_{ion} around 10.6 $\mu\mathrm{K}$ and 100 $\mu\mathrm{K}$ are shown in Fig. 1. For $T_{\mathrm{ion}} \approx 100 \, \mu\mathrm{K}$ we found that in 146 instances out 2×10^5 times, the atoms approached the ion to distances below $R_{\mathrm{w}}/2$, such that they entered the inner regime of the dressed potential. For $T_{\mathrm{ion}} \approx 10.6 \, \mu\mathrm{K}$, the number of atoms entering the inner part of the dressed potential dropped to zero.

IV. DIAGONALIZATION OF THE RYDBERG-ION INTERACTION HAMILTONIAN

In this section we discuss how we calculated the adiabatic atom-ion potential from a direct-diagonalizational approach. The atom-ion potential can within the adiabatic approximation be obtained from the internal level structure of the atom for different but fixed atom ion separations $\mathbf{R}$. Each of those $\mathbf{R}$-dependent energy levels can be viewed as the effective potential between atom and ion, under the assumption, that the internal state follows the corresponding eigenstate adiabatically [2]. We focus on the potential or channel, which correspond to the atom's ground state at infinite separation. The relevant shifts of the ground state will with the parameters we choose and for separations larger than $\sim 0.2 \, \mu\mathrm{m}$ result from the off-resonant coupling to the Rydberg manifold, as can be seen from the simpler perturbational approach discussed in the main text. Therefore, we neglect the effect of the ion's electric field on the ground state level for now keeping in mind that the resulting potential will be a good approximation just in the range considered above. For the Rydberg manifold on the other hand the presence of the ion leads to relevant corrections, since it introduces strong couplings between the Rydberg states due to the large polarizability $\alpha \propto n^7$ of the Rydberg states, with n the principal quantum number. Therefore, we model the Hamiltonian representing the atom's internal structure by a single ground state $|gS\rangle$ with energy $\mathcal{E}_{gS}$, which we assume to be unaffected by the ion's electric field, coupled by the dressing laser field to a set of Rydberg states, which are affected by the ion field. With those considerations the Hamiltonian representing the atom's internal structure in the presence of ion and dressing laser reads
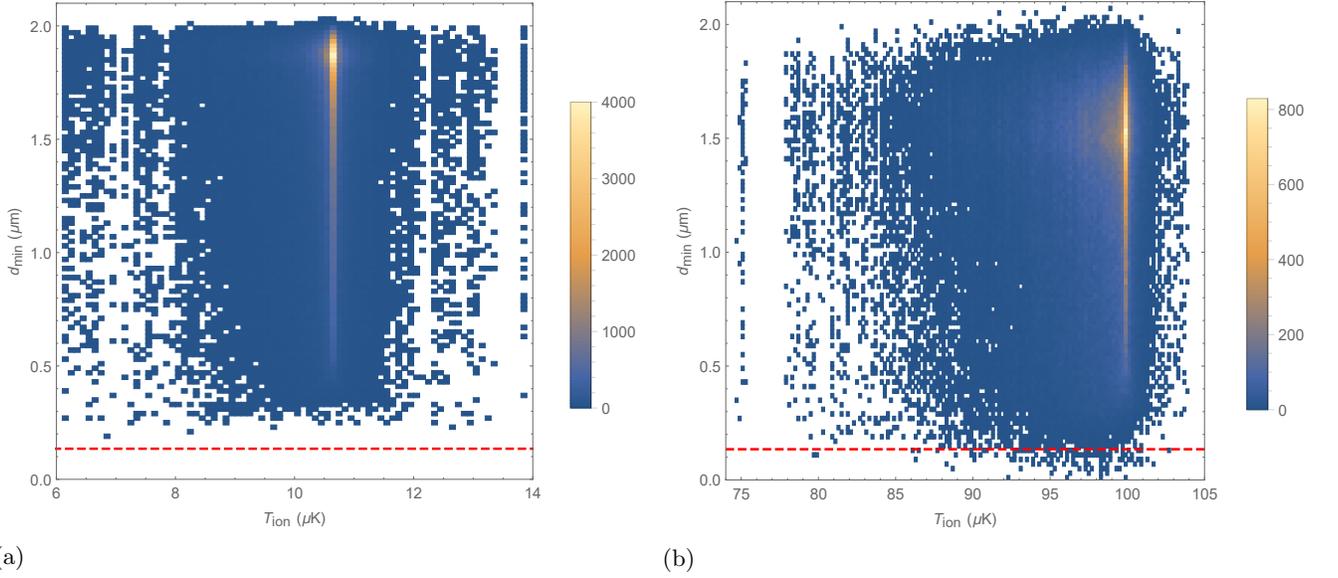
FIG. 1: Ion temperature T_{ion} vs. minimal atom-ion separation d_{min} for 2×10^5 collision simulations of Rb and Yb$^+$ as described in the main text with (a) T_{ion} around 10.6 μK and (b) T_{ion} around 100 μK. The dashed line indicates $R_{\text{w}}/2$, where the atoms find themselves within the inner part of the dressed potential.

$$\hat{H} = \hat{H}_{gS} + \hat{H}_{Ryd} + \hat{H}_{ia} + \hat{H}_L, \tag{9}$$

where $\hat{H}_{gS}$ describes the unperturbed atomic ground state $|gS\rangle$ and is given by:

$$\hat{H}_{gS} = \mathcal{E}_{gS}|gS\rangle\langle gS|. \tag{10}$$

$\hat{H}_{\text{Ryd}}$ represents a set of unperturbed atomic Rydberg states in diagonal form, which in quantum defect theory [3] can be represented by a single Rydberg electron and a singly charged atomic core, which represents the inner electrons and the nucleus:

$$\hat{H}_{Ryd} = \sum_k \mathcal{E}_k |k\rangle\langle k|, \tag{11}$$

where k represents the tuple of quantum numbers (n, l, j, m_j) ranging over the common hydrogen fine structure states and $\mathcal{E}_k$ is the corresponding Rydberg energy level with eigenstate $|k\rangle$ in the relative Rydberg electron-core variable. We obtained those eigenenergies and states in coordinate representation employing the Numerov method and quantum defects found in literature [3].

$\hat{H}_{\text{ia}}$ comprises the interaction terms between Rydberg atom and ion in the quantum defect theory approach. It consists of two Coulomb interaction terms V_C, a repulsive one between ion and atomic core and an attractive one between ion and Rydberg electron. In addition, we included a spin-orbit like coupling term V_{SO}^{e-i} representing the coupling of the ion's electric field to the spin of the Rydberg electron [2].

$$
\begin{aligned}
\hat{H}_{ia} =& V_C(\mathbf{r}_c - \mathbf{r}_i) - V_C(\mathbf{r}_e - \mathbf{r}_i) + V_{SO}^{e-i} \\
=& -\frac{e^2}{4\pi\epsilon_0|\mathbf{R} + \frac{m_c}{M}\mathbf{r}|} + \frac{e^2}{4\pi\epsilon_0|\mathbf{R} - \frac{m_e}{M}\mathbf{r}|} - \frac{1}{2m_e^2c^2}\hat{\mathbf{S}} \cdot \left(\left(\frac{e^2(\mathbf{R} + \frac{m_c}{M}\mathbf{r})}{4\pi\epsilon_0|\mathbf{R} + \frac{m_c}{M}\mathbf{r}|^3}\right) \times \mathbf{p}\right) \\
\approx& \frac{e^2}{4\pi\epsilon_0|\mathbf{R}|^3}\left(-\mathbf{r}\cdot\mathbf{R} + \frac{m_c - m_e}{2M}\mathbf{r}^2\right) - \frac{3e^2(m_c - m_e)}{8\pi\epsilon_0 M|\mathbf{R}|^5}(\mathbf{r}\cdot\mathbf{R})^2 - i\frac{e^2\mu}{4\pi\epsilon_0\hbar m_e^2c^2}\frac{1}{|\mathbf{R}|^3}\hat{\mathbf{S}} \cdot (\mathbf{R} \times [\hat{H}_{Ryd}, \mathbf{r}]).
\end{aligned} \tag{12}
$$

Here $\mathbf{r}_i$, $\mathbf{r}_c$ and $\mathbf{r}_e$ are the ion, core and Rydberg electron position operators in the laboratory frame respectively, $\mathbf{r}$ and $\mathbf{p}$ are the relative position and relative momentum operator between core and Rydberg electron, $\hat{\mathbf{S}}$ is the

spin-1/2 operator of the electron, e denotes the elementary charge, m_e and m_c denote the electron and core mass respectively, M and μ are the total and reduced mass of the atom respectively and ϵ_0 is the vacuum permittivity. The approximation has been obtained by taylor expanding the terms and substituting the momentum operator in the last term with $\mathbf{p} \approx i2\frac{\mu}{\hbar}[\hat{H}_{Ryd}, \mathbf{r}]$ [2]. The approximation includes terms up to quadrupole order in the Coulombic terms taking account for the non-linearity of the potential over the spatial extent of the Rydberg wavefunctions considered. The term $\hat{H}_L$ of Eq. 9 describes the dressing laser field in dipole approximation, which couples the Rydberg states off-resonantly to the ground state $|gS\rangle$.

$$\hat{H}_L = \sum_k e^{i\omega_L t}\Omega_{(k,gS)}|gS\rangle\langle k| + h.c. \tag{13}$$

where $\Omega_{(k,gS)}$ denotes the Rabi frequency of the transition $|k\rangle$ to $|gS\rangle$ and the sum runs over all Rydberg states $(k) = (n,P,j,m_j)$ for which the transition is dipole allowed.

We proceed in changing to a rotating frame of the ground state with respect to the dressing laser frequency and perform a rotating wave approximation. This affects only $\hat{H}_{gS}$ and $\hat{H}_L$, which transform to

$$\hat{H}'_{gS} = (\mathcal{E}_{gS} + h\omega_L)|gS\rangle\langle gS|$$
$$\hat{H}'_L = \sum_k \Omega_{(k,gS)}|gS\rangle\langle k| + h.c. \tag{14}$$

To determine the coupling strengths $\Omega_{((n,P,j,m_j),gS)}$ we computed the transition matrixelements with an approximate solution for the ground state wavefunction, which we obtained as in the Rydberg case. We restrict to the case of linear polarization along the direction of the ion electric field and fix the couplings such that they are consistent with the case that neglects the fine structure in the main text, namely $\Omega_{(19P,gS)} = 2\pi\,200$ MHz. To this end, we rescaled the couplings such that $\Omega_{((19,P,3/2),gS)} = \Omega_{(19P,gS)}A_{FS}/A$, with $A = \langle P, m_l = 0|\cos(\theta)|S, m_l = 0\rangle$ and $A_{FS} = \langle P, j = 3/2|\cos(\theta)|S, j = 1/2\rangle$ the angular component of the dipole operator coupling angular and fine structure base states respectively. The couplings obtained in this way were found to be in agreement with the scaling law $\Omega_{((n,P,j),gS)} \propto n^*(n,P,j)^{-3/2}$ with $n^*(n,l,j) = n - \delta_{nlj}$ and δ_{nlj} the quantum defects. Diagonalization for $n = 10..30$ and $\omega_L = (\mathcal{E}_{(19,S,1/2)} - \mathcal{E}_{gS})/h + \Delta$ results in the potential shown in Fig. 2 of the main text.

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