Controlling ultracold chemical reactions via Rydberg-dressed interactions

Jia Wang,1 Jason N. Byrd,1,2 Ion Simbotin,1 and R. Côté1,3

1Department of Physics, University of Connecticut, 2152 Hillside Rd., Storrs, CT 06269, USA
2Quantum Theory Project, University of Florida, Gainesville, FL 32611
3Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

We show that ultracold chemical reactions can be manipulated and controlled by using Rydberg-dressed interactions. Scattering in the ultracold regime is sensitive to long-range interactions, especially when weakly bound (or quasi-bound) states exist near the collision threshold. We investigate how, by Rydberg-dressing a reactant, one enhances its polarizability and modifies the long-range van der Waals collision complex, which can alter chemical reaction rates by shifting the position of near threshold bound states. We carry out a full quantum mechanical scattering calculation for the benchmark system H2+D, and show that resonances can be moved substantially and that rate coefficients at cold and ultracold temperatures can be increased by several orders of magnitude.

A key advantage of ultracold systems is the extraordinary degree of control they provide, such as tunable interactions through Feshbach resonances [1] used to investigate degenerate quantum gases [2,4]. This control allows to probe exotic three-body Efimov states [5], and to study ultracold molecules [6,7] and modify their chemistry [8,10], e.g., by orienting them [9,11]. Another approach to modify interactions is to excite atoms into Rydberg states [12], where they acquire extreme properties (e.g., long lifetimes or large electric dipole moment) [13]: long-range Rydberg trilobite molecules [14,15] or macrodimers [16,17] exemplify these exaggerated properties. The control over strong interactions led to proposals for quantum computing [18], e.g., to achieve quantum gates [19,20] or study quantum random walks [21], and to the excitation blockade mechanism [22], where a Rydberg atom prevents the excitation of nearby atoms [12,23,26]; this effect is used to realize electromagnetically induced transparency [24,25] to generate single photons [29] and photon-photon interactions [30,31], or non-destructive imaging of Rydberg atoms [32] to study dynamics of energy transport [33].

Recent studies propose using Rydberg dressing to explore many-body physics [34,35] such as dipolar BEC [36], supersolid vortex crystals in BEC [37] and to cool polar molecules [38]. In this letter, we show how ultracold chemical reactions can be modified and controlled by Rydberg-dressing an atom approaching a diatom, which increases its polarizability and modifies the atom-diatom van der Waals complex and the reaction rate. We consider H2+D, a benchmark system for quantum calculations explored extensively at ultralow [39] and higher temperatures [40], and for which accurate ab initio potential energy surfaces (PES) [11,12] exist. Here, the deuterium atom D is Rydberg-dressed by weakly coupling its ground state |g⟩ to a Rydberg state |r⟩ of width γr using a far detuned continuous-wave (CW) linearly polarized laser (see Fig. 1a)). At large separation, when the atom-molecule interaction is negligible, the atom can be modeled as a two-level system. The CW laser, described by an oscillating electric field $\mathcal{E}\cos\omegaLt$ of strength $\mathcal{E}$ and frequency $\omega_L$, couples $|g⟩$ (energy $E_g$) and $|r⟩$ (energy $E_r$) with Rabi frequency $\hbar\Omega = \langle g | \mu | r \rangle$, (µ: dipole transition moment). The detuning $\delta$ is defined by $\hbar\delta = \hbar\omega_L - (E_r - E_g)$.

Under far-detuning ($|\delta| \gg |\Omega|$) and low laser power ($|\Omega| \ll |\delta|$), conditions, the state of the atom (up to a global phase) within the rotating wave approximation (RWA) is $|a⟩ \approx \sqrt{1 - |b|^2}|g⟩ + |b⟩|r⟩$, where $b = \frac{1}{\sqrt{2}}(\Omega/\delta)e^{-i(\omega_L t - \phi_0)}$, and $\phi_0$ is an initial phase. Properties of dressed atom can be obtained using $|a⟩$; e.g., its dynamic polarizability $\alpha(\omega)$ and dipole moment $d_a$

$$\alpha_a(\omega) = (1 - |b|^2) \alpha_a^{(g)}(\omega) + |b|^2 \alpha_a^{(r)}(\omega), \quad (1)$$

$$d_a = (1 - |b|^2) d_a^{(g)} + |b|^2 d_a^{(r)}, \quad (2)$$

where $\alpha_a^{(j)}(\omega) = \sum_{k \neq j} \frac{2\omega_{jk}|\mu|^2}{\hbar^2(\omega_{jk} - \omega)^2}$ and $d_a^{(j)} = \langle j | \mu | j \rangle$ are
the dynamic polarizability and dipole moment of the atom in state \(|j\rangle\), respectively: \(\hbar\omega_{jk} = E_k - E_j\), and the fast oscillating cross terms containing \(|g|\mu|r\rangle\) are neglected. The static polarizability \(\alpha^{(s)}_n(0)\) for Rydberg states is usually much larger than that of the ground state \(\alpha^{(s)}_6(0)\) (since \(\hbar\omega_{jk}\) can be small). A linearly polarized laser can excite D (or an alkali atom) from its atomic \(s\) ground state into a Rydberg state \(|j\rangle = |n, \ell_e, m_e\rangle\) (with principle quantum number \(n\), electron angular momentum \(\ell_e = 1\) with projection \(m_e = 0\)); Fig. 4(b) shows the rapid growth of \(\alpha^{(s)}(0)\) for the \(np\) state of D (\(n \leq 10\)). Note that without external fields mixing states of different parities, \(d^{(r)}_6 = 0\) (e.g., for D in a pure \(np\) state).

While \(d^{(r)}_6\) remains small, even a weak electric field leads to Stark splittings of Rydberg states: in the linear Stark regime, the highest state of a given manifold \(n\) has a large dipole moment \(d^{(s)}_6 = \frac{3}{2} n(n-1)\) a.u. \[3\]. Even with a small mixing \(|b|^2 = |\Omega/\delta|^2/4\), a Rydberg-dressed atom can still possess a large polarizability (see Fig. 4(c)) and in some cases a large dipole moment which determine the long-range interaction with another atom or molecule.

In Fig. 2(a), we show the PES’s dependence on the reaction coordinates (i.e. the distance between H2 and D in the entrance channel, and HD and H in the exit channels). Rydberg-dressing D changes the long-range interaction in the entrance channel; for H2 in its ground electronic state (no permanent dipole moment), the leading interaction \(-C_6/R^6\) depends on the van der Waals coefficient \(C_6\). Here, we assume the distance \(R\) between D and H2 is large enough, and neglect the anisotropy of H2. Note that if the molecule has a permanent dipole moment (e.g., for heteronuclear molecules) and the atom is Rydberg dressed to a Stark state, the leading interaction is the dipole-dipole interaction. Two components contribute to \(C_6 = C_6^{(ind)} + C_6^{(dis)}\), a dipole induced-dipole term \(C_6^{(ind)}\) \(\propto d^2_6\), and a dispersion term \(C_6^{(dis)}\) \(\propto \alpha_a\).

By changing \(\alpha_a\) and \(d_6\) using Rydberg-dressing, one can modify the long-range atom-molecule van der Waals complex, and affect scattering properties.

The dispersion term \(C_6^{(dis)}\) for an atom in state \(|j\rangle\) can be evaluated by the Casimir-Polder integral

\[
C_6^{(dis)} = \frac{3}{\pi} \int_0^\infty \alpha_m(i\omega)\alpha_a(j)(i\omega)d\omega,
\]

where \(\alpha_m\) and \(\alpha_a\) are the dynamical polarizability of the molecule and of the atom, respectively. Inserting Eq. 1 into the Casimir-Polder integral gives

\[
C_6^{(dis)} = C_6^{(g,dis)} + |b|^2 \Delta C_6^{(r,dis)},
\]

where \(\Delta C_6^{(r,dis)} \equiv C_6^{(r,dis)} - C_6^{(g,dis)}\). The corresponding induction term is \(C_6^{(ind)} = \frac{3}{d^2_6} C_6^{(j,ind)}\), where \(\alpha_{pq}\) is the \(pq\) component of the cartesian static molecular dipole polarizability tensor (with \(z\) along the molecular symmetry-axis). Inserting Eq. 2 and noting that \(d^{(r)}_6 = 0\), we find \(C_6^{(ind)} = |b|^4 C_6^{(r,ind)}\).

The components of \(C_6\) for the benchmark system H2+D, tabulated in Table I show a rapid increase with \(n\). They were computed using the TD-DFT/vdW method \[43\] developed to obtain the dynamic polarizability for H2 using the large aug-cc-pVTZ basis set \[14\] and the PBE0 density function. The dynamic polarizability of D was computed using Gauss-Laguerre quadrature, where the integration grid and number of excited states (computed using the proper reduced mass for D) was converged to provide an accuracy better than 0.1% (continuum contributions were omitted for D, suggesting a 5-10% underestimate of \(C_6^{(r,dis)}\)). \(C_6\) was computed using gaussian quadrature, with the induced term calculated for the highest Stark-splitled state for a given \(n\).

In our benchmark example H2+D, we consider dressing D with a CW laser blue-detuned (\(\delta > 0\)) from 3p
To compute the effect of Rydberg-dressing on chemical reactions, we adopted the H$_2$+D electronic ground PES of Ref. [11], already tested at ultracold temperatures [39]. The potential $V(r) \equiv V(r_{12}, r_{23}, r_{31})$ depends on the internuclear distances $r \equiv \{r_{12}, r_{23}, r_{31}\}$, where 1 stands for D, and 2 and 3 for the two identical H atoms. The distances between H$_2$ and D then is simply given as $R = \frac{1}{2}(r_{12}^2 + r_{23}^2 - r_{31}^2)$. Similar to Eq. (10), the three-body surface of H$_2$ interacting with a blue-detuned Rydberg-dressed D atom can be written as

$$\tilde{V}(r) = V(r) + \Delta(R) ,$$

where the blue-detuning ensure the smooth transition from the dressed long-range PES to the bare PES at shorter $R$ without incurring possible avoided-crossing for red-detunings [45]. We choose $b$ so that the transition occurs far enough from the van der Waals complex well (minimum of the blue curve in Fig. 1). We obtain the $S$-matrix by performing a fully quantum mechanic scattering calculation using the ABC code of Manolopoulos and coworkers [46] modified for the ultracold regime [33, 47]. The state-to-state cross sections are given by

$$\sigma_{q'q}(E) = \frac{\pi}{k_{q'}^2 (2j + 1)} \sum_{\ell, q} |\delta_q'q - S^j_{q'q} \sigma_q(E)|^2 ,$$

where $q = \{a, v, j\}$ is the set quantum numbers describing the molecular state (vibration $v$, rotation $j$, and arrangement $a$): $a$ distinguishes the final state H$_2$+D (quenching) from HD+H (reaction). $J$ is the three-body total angular quantum number, and $\ell$ indicates the relative angular momentum between the initial reactants H$_2$ and D. The scattering wave number $k_q$ is defined by

$$h^2 k_q^2 = E_c = 2\mu_{H_2+D} [E - (\varepsilon_{v,j} + |b|^2h\delta)] ,$$

where $E_c$ is the collisional energy and $\varepsilon_{v,j}$ is the initial rovibrational energy of H$_2$ (in state $\{v, j\}$), $|b|^2 h\delta$ corresponds to the shift due to the Rydberg dressing shown in Eq. (7), and $\mu_{H_2+D} = m_{H_2} + m_D$ is the reduced mass. We define the total energy-dependent inelastic rate as

$$\kappa_{in}(E) = v_{rel} \sum_{J'\neq q} (2J + 1) \sigma_{J'q}(E) ,$$

where $v_{rel} = h k_{q} / \mu_{H_2+D}$ is the relative velocity. The sum is over all final channels but the entrance channel. Quenching/reaction rates ($\kappa_{V/R}$) are obtained by splitting the sum with $a' = a$ and $a' \neq a$, respectively [32].

Numerical results for $\kappa_{in}$ in the “bare” case ($|b| = 0$) for H$_2$($v = 0, 1, 2, j = 0$)+D are shown in Fig. 3(a). Resonances occur for both $v = 0$ and 1, but not 2: the s-wave ($\ell = 0$) and p-wave ($\ell = 1$) components are also shown, revealing the p-wave nature of these resonances. By varying the amount of Rydberg-dressing $|b|$, the resonances can be moved substantially, while the non-resonant $v = 2$ is only slightly affected. In these calculations, we fix

(Fig. 2(b)) to prevent populating the Rydberg state; as D approaches H$_2$, the detuning increases leading to a weaker effect. For simplicity, we also consider no static field and omit $C_6^{(\text{ind})}$; we can then drop the superscript (dis) and write $C_6 = C_6^{(g)} + |b|^2 \Delta C_6^{(r)}$. Within the RWA, the Hamiltonian for the internal degrees of freedom at a fixed large separation $R$ can be written as a $2 \times 2$ matrix (in the basis $|am\rangle \equiv |a \rangle \otimes |m\rangle$ where $|a\rangle = |g\rangle$ or $|r\rangle$ is the atomic state, and $|m\rangle$ the state of the molecule):

$$H = \begin{pmatrix}
-C_6^{(g)} / R^6 & \hbar \Omega / 2 \\
\hbar \Omega / 2 & -h\delta - C_6^{(r)} / R^6
\end{pmatrix} ,$$

where the ground state atom-molecule collision threshold is set to zero. By diagonalizing $H$, we obtain two Born-Oppenheimer curves: a dressed ground curve $U_g$ between H$_2$ and ground-state D (dressed by $|r\rangle$), and a dressed excited curve $U_e$ between H$_2$ and excited D (dressed by $|g\rangle$). Assuming $|\Omega / \delta| \ll 1$ and $C_6^{(r)} > C_6^{(g)}$, we find

$$U_g(R) = -C_6^{(g)} / R^6 + \Delta(R), \quad \text{with } \Delta(R) = \frac{\hbar \Omega}{4 |\delta(R)|} ,$$

where $\hbar \Omega = \hbar \Omega + \Delta C_6^{(r)} / R^6$, with $\Delta C_6^{(r)} = C_6^{(r)} - C_6^{(g)}$. In the large $R$-limit such that $\Delta C_6^{(r)} / R^6 \ll |\delta(R)|$, the long-range behavior of $U_g(R)$ is given by

$$U_g(R) \to -C_6^{(g)} / R^6 + |b|^2 \delta C_6^{(r)} / R^6 + |b|^2 h\delta = -C_6^{(g)} / R^6 - |b|^2 h\delta ,$$

where $b = \Omega / (2 \delta)$ is the mixing parameter defined before. In Eq. 7, the first term is a change of the effective $C_6$ due to Rydberg-dressing, which agrees with the result discussed before, and the second term represents a shift of the collision threshold (absent in our previous discussion). At shorter distance where $\Delta C_6^{(r)} / R^6 \gg |\delta(R)|$, the term $\Delta(R)$ becomes negligible compared to $C_6^{(g)} / R^6$ in Eq. 8 as it smoothly goes to zero; only the long-range part of the interaction is modified by the blue-detuned Rydberg-dressing field. The transition between the two regimes is shown in Fig. 2(c).

Similarly, the curve between the Rydberg atom and the molecule is dressed by the laser, effectively shifted down by $\Delta(R)$: (with $|\Omega / \delta| \ll 1$ and $C_6^{(r)} > C_6^{(g)}$)

$$U_e(R) = -C_6^{(r)} / R^6 - h\delta - \Delta(R) ,$$

which, in the large $R$-limit ($\Delta C_6^{(r)} / R^6 \ll |\delta(R)|$), becomes

$$U_e(R) \to -C_6^{(r)} / R^6 - |b|^2 \delta C_6^{(r)} / R^6 - (1 + |b|^2) h\delta .$$

This implies smaller slightly effective van der Waals coefficient and slightly larger effective detuning.
\[
\delta \approx 296.09 \times 2\pi \text{ GHz}, \text{so that the threshold shift } |b|^2 \hbar \delta \text{ of } U_g \text{ affects the position of the bound state in the entrance arrangement of the van der Waals complex. Even a modest } |b| \text{ is sufficient to move a resonance significantly (cases } v = 0 \text{ and } 1), \text{ while much larger values are required if the van der Waals complex is not just about to support a new bound-state (} v = 2). \text{ Thus we limit our investigation to values of } |b| = \Omega/(2\delta) \leq 0.1, \text{ implying a laser intensity less than } 3 \times 10^8 \text{ W/cm}^2. \text{ The } v = 1 \text{ level is particularly sensitive to a weak amount of Rydberg-dressing, with the resonance having a larger magnitude and moving to much lower energy for } |b| = 0.03, \text{ and simply disappearing for a slightly larger } |b| \approx 0.04, \text{ when the quasi-bound state in the van der Waals complex becomes bound. Figure } 3(b) \text{ compares the bare } \kappa_{in}(v = 0) \text{ with its thermal average (using a Maxwell distribution of } \kappa_{rel} \text{ characterized by a temperature } T) \text{: the agreement between both will become better as the resonance moves to lower } E_c. \]

Figure 4 shows this sensitivity of \( \kappa_{in} \) (\( v = 1 \)) by varying \( |b| \) and \( E_c \); as \( |b| \) increases, the resonance shifts to lower \( E_c \) with an increased magnitude until it disappears near \( |b| \approx 0.04 \), at which point the van der Waals complex acquires a new bound-state. As \( |b| \) increases still, the maximum in \( \kappa_{in} \) starts shifting to larger \( E_c \) with a decreasing magnitude. This example shows that one can, with modest Rydberg-dressing, adjust and control \( \kappa_{in} \) in chemically active systems, by not only moving the position of resonances but also increasing their magnitude by several orders. For example, if \( E_c \) (or temperature) of a given experiment is near the resonance, the rate could be reduced by moving the resonance away, or in cases where \( E_c \) is not near the resonance, Rydberg-dressing could move it to the right energy range. The ratio of inelastic to elastic cross sections in Fig. 5(a) shows the sharp increase (near \( |b| \approx 0.03 \)) in relative inelasticity. Note that elastic processes are less relevant from a chemical perspective since reactants stay in their initial states. The branching ratio \( \kappa_2/\kappa_{in} \) for \( v = 1 \) in Fig. 5(b) shows how chemical reactions can be controlled within a factor of two by varying \( |b| \) near 0.03; for \( v = 0 \), where only reaction channels exist, \( \kappa_2/\kappa_{in} \), the reaction rate can be changed by several orders of magnitudes (see Fig. 3). Fig. 5 suggests that the ratios \( \sigma_{in}/\sigma_{el} \) and \( \kappa_R/\kappa_{in} \) can be modified and controlled by Rydberg dressing.

In conclusion, we have shown that ultracold chemical reactions can be manipulated and modified using Rydberg-dressing. Although the concept was illustrated by dressing an atom approaching a diatomic molecule using the benchmark \( \text{H}_2+\text{D} \) system, this approach is general and could be applied to a wide range of systems. If the molecule has a permanent dipole moment, e.g. for the system \( \text{LiH}+\text{H} \), Rydberg-dressing the atom would lead to a long-range interaction dominated by strong dipole induced \( C_6 \) due to the large dipole of \( \text{LiH} \). With additional external electric fields, strong dipole-dipole interaction will become important. These strong long-range interaction might eventually lead to different branch ratios into exit channels. We note that Rydberg-dressing the final
products instead of the reactants might allow one to direct the flux of probability into specific channels, and thus to control the branching ratios for different final channels. This would open up the possibility of state-to-state control of chemical reactions.

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