Long-range interactions between polar alkali-metal diatoms in external electric fields

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We computed the long-range interactions between two identical polar bialkali molecules in their rovibrionic ground level, for all ten species, using accurate quantum chemistry results combined with available spectroscopic data. Huge van der Waals interaction is found for eight species in the free space. The competition of the van der Waals interaction with the dipole-dipole interaction induced by an electric field parallel or perpendicular to the intermolecular axis is described as functions of the electric field magnitude and intermolecular distance. Our calculations predict a regime with a mutual orientation of the two molecules but with no preferential direction in the lab frame. A mechanism for the one-photon assisted association of a pair of ultracold polar molecules into ultracold tetramers is proposed, which would open the way towards the optical manipulation of ultracold polyatomic molecules.

The dynamics of ultracold quantum gases composed of atoms or molecules with extremely low translational energy $E_i/k_B \ll 1$ millikelvin is dominated by the long-range mutual interactions between particles. Such gases are nowadays routinely produced and many applications are foreseen [1, 2]. When they are trapped in external potentials created by electromagnetic fields, they offer unique opportunities to study fundamental few-body dynamics in atomic and molecular physics [3]. The unprecedented capability to simultaneously control the internal and external degrees of freedom of the particles also opens the way to the quantum simulation of Hamiltonians describing many-body physical phenomena like low-temperature Fermi fluids or artificial gauge fields [4, 5]. When the particles possess an intrinsic magnetic or electric dipole moment they interact through strong long-range anisotropic forces, i.e. depending on their mutual orientation, which strongly modifies the dynamics of the quantum gas [6, 7] and enhances stereochemical properties of ultracold bimolecular reactions [8].

The recent production of ultracold heteronuclear alkali-metal dimers in their lowest rovibrionic [8, 10] and hyperfine level [11] stimulates many studies in this perspective. The permanent electric dipole moment (PEDM) $d_0$ of such (polar) molecules in their own frame allows for manipulating them with static electric fields [12, 13] and electromagnetic fields [8, 11, 16]. Such studies require a detailed modeling of the molecule-molecule long-range interactions inside the quantum gas with or without the presence of external fields [17, 18]. The most spectacular experimental achievements on ultracold dipolar molecular gases have been performed on KRb molecules [8, 3, 11, 19] which motivated a wealth of theoretical investigations on this species [17, 20, 22]. An accurate description of long-range interactions involving the other heteronuclear alkali diatoms is strongly needed since they draw rising attention [21, 32]. Considering two identical polar molecules at large distances $R$ between their individual center-of-mass (c-o-m) connected by the $z$ axis and with polar angles $(\theta_i, \phi_i), i = 1, 2$ with respect to the $z$ axis, their mutual long-range dipole-dipole interaction is conveniently written in the coordinate system associated with the tetramer (T-CS) based on the $z$ axis

$$V_{dd}(R) = -\frac{d_0^2}{R^6} (2 \cos \theta_1 \cos \theta_2 - \sin \theta_1 \sin \theta_2 \cos (\phi_2 - \phi_1))$$

In the range of distances investigated here, it is easy to check that the energy of the mechanical rotation between the two molecules, and thus the corresponding rotational couplings, are small compared to the van der Waals (vdW) interaction and to the rotational energy of the individual molecules, so that the main features of the problem can be captured in the T-CS.

In this paper, we compute the long-range interactions between two identical bosonic polar bi-alkali ground state molecules both in free space and as a function of the magnitude of an external electric field parallel or perpendicular to the $z$ axis. We use the stationary perturbation theory as in our previous investigations on atom-molecule systems [23, 24]. In free space, the vdW interaction varying as $-C_6/R^6$ is characterized by $C_6$ coefficients that are three orders of magnitude larger than those for alkali atoms. The isotropic vdW interaction competes with the expected anisotropic dipole-dipole interaction induced by one molecule on the other, or by an external electric field $\mathcal{E}$ [14, 28]. Among the ten species built from Li, Na, K, Rb, and Cs atoms, we show that interactions for KRb and LiNa behave differently from species with a larger PEDM. For the latter molecules, our calculations predict for critical values of $R$ and $\mathcal{E}$ the mutual orientation of the two molecules but with no preferential direction in the lab frame, i.e. no anisotropy of their interaction. Our work complements the one by Byrd et al. [18] where the authors investigated the long-range interaction between two bi-alkali ground state polar molecules aligned by a strong external electric field in the head-to-tail or side-by-side configurations in the lab frame.
In the lowest rovibrational level \((v_1 = v_2 = 0; j_1 = j_2 = 0)\) of their ground electronic state \(X^1\Sigma_g^+\), the molecules have no PEDM in the T-CS. Their interaction energy \(V_{ji}(R)\) is determined by the operator \(\tilde{V}_{dd}\) taken at the second order of the perturbation expansion, i.e. \(-C_6/R^6\). The \(C_6\) coefficient is expressed as \(C_6 = C_6^g + C_6^v + C_6^{g-v}\) \(27\), where the three terms denote the contribution of the electric-dipole-allowed transitions from \((v_i = 0, j_i = 0, i = 1, 2)\) towards higher \(X^1\Sigma_g^+\) levels, towards levels of the electronically-excited states, and a crossed contribution, respectively. We have calculated these terms along the lines described in details in Ref. \(28\). The \(C_6\) coefficients (Table \(1\)) are expressed in terms of dynamic dipole polarizabilities at imaginary frequencies \(39\) extracted from a combination of accurate semi-empirical potential energy curves (PECs) and transition dipole moments (TDMs) computed in our group \(40, 41\), and available spectroscopic PECs. The pure rotational transition \((v_i = 0, j_i = 1) \leftrightarrow (v_i = 0, j_i = 0)\) within \(X^1\Sigma_g^+\) yields by far the dominant contribution to \(C_6^g\) which reduces to a good approximation to \(C_6^g \approx d_0^6/6B_0\) where the rotational constant \(B_0\) of the \(X^1\Sigma_g^+\) \((v_i = 0)\) molecules and \(d_0\) are expressed in atomic units (see Table \(1\)). For eight of the ten species \(C_6^g\) represents more than 87% of the total \(C_6\) which thus reaches values up to three orders of magnitude larger than for KRb and LiNa. Note that the \(C_6^g\) values are comparable to those for homonuclear molecules \(43\), while the crossed terms \(C_6^{g-v}\) are always very weak. Our results are in good agreement with Refs. \(18, 27, 42\) where the chosen molecular data are slightly different and where the molecules are taken at their equilibrium distance. We consider in the following the eight molecules for which \(C_6^g\) is dominant as dipolar rotators (all but KRb and LiNa), ignoring the influence of the excited electronic states in their interaction.

The above single-channel description is valid down to distances \(R^* = (\delta_0^6/B_0)^{1/6}\) such that \(C_6^g/2R^6 \approx 2B_0\) where the dipole-dipole interaction couples the \((j_i = 0)\) and \((j_i = 1)\) levels \(13\). This is easily shown using an analytical model including the two channels \((j_1, j_2) = (0, 1)\), \((1, 1)\). Defining dimensionless energies \(V = V/B_0\) and distances \(\tilde{R} = R/R^*\), the lowest potential energy curve \(\tilde{V}_{0,0}(\tilde{R})\) reads

\[
\tilde{V}_{0,0}(\tilde{R}) \approx 2 - 2\sqrt{1 + 1/6\tilde{R}^6}.
\]  

Thus \(R^*\) is the distance where the variation of \(\tilde{V}_{0,0}\) suddenly changes from a variation in \(\tilde{R}^{-6}\) to \(\tilde{R}^{-3}\) due to the coupling with higher channels (Fig. \(1\)), inducing the mutual alignment of the molecules. As previously found \(28\), the values of \(R^*\) are about two times smaller than the vdW length \(R_{vdW}\) (Table \(1\)) where quantum reflection occurs \(44, 45\). We checked that this sudden change in the interaction does not modify the quantum reflection and thus the universal collision rates defined in Ref. \(28\).

The full formalism must take into account the coupling between rotational levels of the diatoms induced by \(\tilde{V}_{dd}\). (assuming \(v_1 = v_2 = 0\)), by diagonalizing at each \(R\) the Hamiltonian \(\hat{H} = \hat{H}_1 + \hat{H}_2 + \tilde{V}_{dd}\), in the rotational basis \(|\beta\rangle = |j_1m_1j_2m_2\rangle\), with \(m_i\) the projection of \(j_i\) on \(z\), and for a given parity \(p = (-1)^{j_1+j_2}\) and a given \(M = m_1 + m_2\). The free rotation terms \(\hat{H}_i\) of molecule \(i\) only have diagonal elements equal to \(B_0j_1(j_1+1)\). The matrix elements of the dipolar Hamiltonian \(\hat{W}\) read

\[
\langle \beta'|\hat{W}_{dd}|\beta\rangle = \frac{d_0^2}{R^3} C_{ji010}^0 C_{j20j0}^0 \sum_q A_q C_{j11q}^{m_1} C_{j2m21-q}^{m_2},
\]

(3) where \(A_q = -2[(1+q)(1-q)]^{-1}\times[(2j_1+1)(2j_2+1)]^{1/2}\times[(2j'_1+1)(2j'_2+1)]^{-1/2}\) is a numerical factor, and \(C_{\alpha\beta\rho\delta}^{\gamma}\) a Clebsch-Gordan coefficient \(46\). Values up to \(j_i = 6\) for \(R > 10, j_i = 10\) for \(0.25 < R < 10\) and \(j_i = 15\) for \(0.1 < R < 0.25\) have been included in the calculations. In analogy with two atoms, the resulting adiabatic potential energy curves (PECs) are labeled \(|M|\) \(g, p\) where \(\sigma\) is the symmetry with respect to a plane containing the intermolecular axis (Fig. \(1\)). Note the behavior of the lowest \(0_p^{+}(+)\) and \(0_p^{-}(-)\) curves which get closer and closer when \(R\) decreases. This will have important consequences in the presence of an electric field.

In the T-CS the influence of an external electric field on the molecule-molecule interactions is for instance relevant when studying one- and two-dimensional trapping geometries. The field-molecule Hamiltonian \(\hat{W}_i = \hat{\mathcal{E}}_i\) reduces to \((-\mathcal{E}\cos \theta_i)\) and \((-\mathcal{E}\sin \theta_i\cos \phi_i)\) for a parallel (along \(z\), \(\pi = 0 \equiv |0\rangle\)) and perpendicular (along \(x\), \(\pi = 1 \equiv |1\rangle\)) field, respectively. Its matrix elements for molecule 1 (and vice-versa for molecule 2) coupling states with different parity \(p\) and \(p'\) are

\[
\langle \beta'|\hat{W}_1^\pi|\beta\rangle = -\delta_{j_2j_1} \delta_{m_2m_1} \left(\frac{2j_1+1}{2j_2+1}\right) \sum_q C_{ji010}^q C_{j20j0}^q \mathcal{E}_d q.\]

(4)
The lowest PEC is conveniently and computation of the PECs through the diagonalization increases, the barrier shifts toward low $R_1$. The $v_dW$ term competes with a side-by-side repulsive attractive where the energy of the two infinitely separated molecules directly coupled to the $0^+$ state with $g_0 \gg 1 \pi^0$.

The dimensionless quantity $\bar{\mathcal{E}} = \mathcal{E}/\mathcal{E}^*$ holds for the electric field expressed in units of $\mathcal{E}^* = B_0/d$ (Table I).

In the parallel case, the lowest $0_2^{(+)}$ state $|j_1 m_1 j_2 m_2\rangle = |0000\rangle$ is directly coupled to the $0_0^{(-)}$ states $|0010\rangle$ and $|1000\rangle$, while the latter are in turn directly coupled to the $0_2^{(+)}$ state $|1010\rangle$. Similarly, the perpendicular field induces a coupling between the $0_2^{(+)}$ state $|0000\rangle$ with $|0011\rangle$, $|0101\rangle$, $|1100\rangle$, and $|1100\rangle$ which combine together to form $1_1^{(-)}$ states.

A perturbative calculation of the lowest PEC $V_{00;\pi}(\bar{R})$ for $\bar{R} \gg 1$ and $\bar{\mathcal{E}} \ll 1$, including the $(j_1, j_2) = (0, 0), (1, 0), (1, 1)$ channels yields the expression at the third order

$$V_{00;\pi}(\bar{R}, \bar{\mathcal{E}}) \approx (\delta_{\pi 1} - 2\delta_{\pi 0}) \left( \frac{\bar{\mathcal{E}}^2}{9R_0^3} - \frac{1}{6B_0^6} \right) \tag{6}$$

where the energy of the two infinitely separated molecules is set to 0 for each $\bar{\mathcal{E}}$ in the following. For $\pi = 0$ the attractive $R^{-3}$ character of the lowest PEC, induced by the head-to-tail configuration of the two molecules, is valid only for distances such that $\bar{R} \gg \bar{\mathcal{E}}^{-2/3}$, while below this limit the vdW term is dominant. For $\pi = 1$ the “huge” vdW term competes with a side-by-side repulsive $R^{-3}$ term, resulting in an expected potential barrier located at $R_0 \approx (3/\bar{\mathcal{E}}^2)^{1/3}$ with the height $V_{00;\perp} \approx \bar{\mathcal{E}}^4/54$. As $\bar{\mathcal{E}}$ increases, the barrier shifts toward low $R$, but its height remains small compared to $B_0$, even for moderate fields $\bar{\mathcal{E}} \approx 1$.

These features are observable from the full numerical computation of the PECs through the diagonalization of the molecule-molecule + molecule-field Hamiltonians (Eqs. [3] and [4]). The lowest PEC is conveniently and unambiguously characterized by several quantities represented as contour plots in Figs. 2: (i) the leading exponent $n^*(\bar{R}, \bar{\mathcal{E}})$ of the long-range interaction depending on $\bar{R}$ and $\bar{\mathcal{E}}$

$$n^*(\bar{R}, \bar{\mathcal{E}}) = \frac{\partial \log V_{00;\pi}(\bar{R}, \bar{\mathcal{E}})}{\partial \log \bar{R}} \tag{7}$$

(ii) the induced dipole moment $\bar{d}_i(\bar{R}, \bar{\mathcal{E}})$ (in units of $d_0$) along the electric field axis, and (iii) the mutual alignment of the two molecules $s(\bar{R}, \bar{\mathcal{E}})$, expressed as the scalar products

$$\bar{d}_i(\bar{R}, \bar{\mathcal{E}}) = \langle \hat{d}_i \cdot \hat{\mathcal{E}} \rangle, s(\bar{R}, \bar{\mathcal{E}}) = \langle \hat{d}_1 \cdot \hat{d}_2 \rangle \tag{8}$$

where $\langle \ldots \rangle$ denotes the average over the eigenvector associated with the lowest PEC. Several regions can be distinguished in Fig. 2c, e, g of for parallel field. Region III in panel (c) displays the expected $R^{-3}$ attractive behavior of the interaction between two dipoles when they tend to approach each other head-to-tail in an electric field. However panels (c) and (g) show that for low fields ($\bar{\mathcal{E}} < 1$, see III-A) the dipoles are not aligned along the field and average to zero, neither they are aligned against each other, while the inverted situation takes place at high fields ($\bar{\mathcal{E}} > 1$, see III-B). Region III spreads to the low-$R$ values with increasing fields, and its border with region I scales as $\mathcal{E} \sim R^{-1/2}$, as predicted by Eq. (5). The vdW interaction is dominant in Region I, hence the $R^{-6}$ behavior predicted in Eq. (5). Since the molecules have no privileged orientation, $d_1$ and $s$ are both zero. In panel (c) Region I shares its low-$R$ border with Region II, which exhibits a $R^{-3}$ character, corresponding to the alignment of the dipoles again each other (panel (g)) and along the field (panel (e)). Surprisingly this border is independent of the $\bar{\mathcal{E}}$ magnitude, which is related to the almost complete energy degeneracy (for $R \leq 0.5$) of the lowest $0_2^{(+)}$ PEC with the $0_0^{(-)}$ already quoted in Fig. 11 in the field-free case. Thus the two states are strongly coupled even by a small parallel electric field.

| $d_0$ (a.u.) | $B_0$ (cm$^{-1}$) | $C_6$ (a.u.) | $C_{6g}^g/C_6$ (a.u.) | $C_{6g}^g$ (a.u.) | $R_{vdW}$ (a.u.) | $R^*$ (kV/cm) | $\mathcal{E}^*$ (mK) | $R_0$ (a.u.) |
|-------------|----------------|--------------|---------------------|----------------|----------------|---------------|----------------|----------------|
| $^{23}\text{Na}^{133}\text{Cs}$ | 1.845 | 0.058 | 7323100 | - | 0.902 | 9311100 | 574 | 234 | 0.328 | 378 | 5.3 | 12 |
| $^{7}\text{Li}^{133}\text{Cs}$ | 2.201 | 0.187 | 4585400 | 4210000 | 27 | 0.902 | 4574400 | 497 | 178 | 2.0 | 408 | 0.3 | 10 |
| $^{23}\text{Na}^{87}\text{Rb}$ | 1.304 | 0.070 | 1524900 | - | 0.994 | 1515800 | 355 | 175 | 1.3 | 294 | 0.8 | 16 |
| $^{7}\text{Li}^{87}\text{Rb}$ | 1.645 | 0.215 | 1252300 | 1170000 | 27 | 0.994 | 1244200 | 325 | 140 | 3.1 | 428 | 0.6 | 13 |
| $^{7}\text{Li}^{39}\text{K}$ | 1.410 | 0.256 | 570190 | 550000 | 27 | 0.988 | 565300 | 223 | 119 | 4.3 | 169 | 0.02 | 15 |
| $^{23}\text{Na}^{39}\text{K}$ | 1.095 | 0.095 | 561070 | - | 0.987 | 553520 | 240 | 140 | 2.0 | 327 | 0.1 | 19 |
| $^{39}\text{K}^{133}\text{Cs}$ | 0.724 | 0.030 | 345740 | - | 0.953 | 329510 | 274 | 156 | 1.0 | 226 | 0.8 | 38 |
| $^{87}\text{Rb}^{133}\text{Cs}$ | 0.490 | 0.016 | 147260 | 142129 | 42 | 0.879 | 129250 | 236 | 148 | 0.8 | 189 | 1.0 | 60 |

| $^{39}\text{K}^{87}\text{Rb}$ | 0.242 | 0.038 | 15972 | 16133 | 42 | 0.209 | 3336 | 118 | 70 | 4.0 | 451 | 6.10$^{-4}$ | 109 |
| $^{7}\text{Li}^{39}\text{Na}$ | 0.223 | 0.374 | 3583 | 3917 | 27 | 0.067 | 241 | 57 | 31 | 36.1 | 1130 | 6.10$^{-7}$ | 95 |

TABLE I. Permanent dipole moment $d_0$ and rotational constant $B_0$ from Ref. [48] for ground-state molecules in $v = 0$; total $C_6$ and partial $C_{6g}^g$ coefficients for two identical ground-state molecules in the $(v = 0, j = 0)$ level; various characteristic distances (see text) $R_{vdW}$, $R^*$, $R_0$, and position of the barrier ($R_b$, $V_b$) for a field $\mathcal{E} = 1$ kV/cm.
A similar analysis holds also for a perpendicular field (panels d, f, h of Fig. 2). The expected \( R^{-3} \) repulsive behavior of the interaction between two dipoles approaching side-by-side is visible in Region III (panel d), separated from Region I by an irrelevant region (between the dashed lines) due to the divergence of \( n^* \) when the PEC becomes attractive. It turns into an attractive \( R^{-6} \) pattern in Region I while the dipoles are mutually aligned in Regions III-A and II just like in the parallel case. Quite surprisingly in contrast, the mutual interaction between the dipoles is always stronger than their individual interaction with the field so that they are never aligned along the field even at low \( R \) in Region II (panel f).

Fig. 2(a, b) depicts the approximate values of \( n^* \) for the specific case of KRb (but also valid for LiNa) obtained by diagonalizing Eq. 3 in physical units, and adding the diagonal contribution \( -(C_6^p + C_6^q)/R^6 \). It is striking to see that while Regions I and III are similar to those of the former case, the vdW interaction dominates even at short distances (Region II) even at high electric fields, due to the low value of the PEDM.

Table I summarizes the characteristic quantities introduced in this paper. It confirms that the molecules showing a “huge” \( C_6^p \) coefficient are easier to align than LiNa and KRb: they have smaller \( \mathcal{E}^* \) and \( R_0 \) values due to their important permanent dipole moment with a field-induced \( R^{-3} \) character spreading faster for molecules like NaCs. The potential energy height increases with \( C_6^q \) so that colliding molecules like NaCs are unlikely to overcome that barrier in the ultracold regime. Figs. 2(c) and (d) show that a good alignment can be obtained for a field roughly equal to \( 2\mathcal{E}^* \) which requires particular attention for LiK, LiRb and KRb (6–9 kV/cm) and LiNa.

In Ref. 18, the authors compute the terms of the multipolar expansion from \( R^{-3} \) to \( R^{-8} \), for two polar bialkali molecules with fixed distances and angles. Then those purely electronic terms are averaged on electric-field-dressed rotational levels of each molecules, for different intermolecular distances. It is shown that the quadrupole-quadrupole interaction scaling as \( R^{-5} \) dominates the dipole-dipole interaction for distances lower than \( R_q \) (last column of Table I). For the six most polar molecules, \( R_q \) is smaller than 20 a.u., where our model is not valid any more. For LiNa, KRb, RbCs and KCs, this interaction may play a significant role in the small-\( R \) region [17, 18], but it will certainly not alter the general description of the present paper.

The induced electric dipole moment (EDM) of each molecule along the parallel electric field axis (Fig. 2(e)) is non-zero in the T-CS and strongly varies with \( R \) at moderate electric fields (say \( \approx 0.1\mathcal{E}^* \), see the horizontal line in panels (e) and (f)), it changes from \( d = 0.18 \) at \( R = 0.74 \) up to \( d = 0.81 \) at \( R = 0.45 \). For the five species among the ten heteronuclear bialkali molecules which are found stable against ground state collisions (NaK, NaRb, NaCs, KCs, and RbCs) [17], this feature suggests that one-photon-assisted formation of ultracold polar tetramers (with an induced EDM \( \approx 2d \)) could be possible by stimulated radiative association process along the lines proposed in Ref. [48]. In contrast, while being mutually aligned, the individual EDMs induced by an orthogonal electric field in the T-CS average to 0 (Fig. 2(f)) so that such a photoassociation process would not be allowed in such a configuration. This result is relevant for the control of photoassociation of dipolar molecules trapped in 2D optical lattice, opening the way toward the optical manipulation of ultracold polyatomic molecules.

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FIG. 2. The molecule-molecule interaction for the \( \sigma_0^{(+)} \) state \( |0000\rangle \) in parallel (upper row) and perpendicular (lower row) electric field in the T-CS as functions of \( R \) and \( \mathcal{E} \) in reduced units. The color scale ranges from black (minimal values) to white (maximal values). (a)-(b) leading \( n^* \) exponent (Eq. (7)) for KRb; (c)-(d) leading \( n^* \) exponent for all species but KRb and LiNa; (e)-(f) induced dipole moment \( \delta_i \) of molecule \( i \) (\( i = 1 \) or \( 2 \)) along the field axis (Eq. (5)); (g)-(h) scalar product \( s \) of the two dipole moments (Eq. (5)). In (b) and (d) the \(+/-\) symbols refer to a repulsive/attractive interaction, while the zones between the dashed lines are physically irrelevant (see text). The horizontal line in (e) and (f) drawn at \( \mathcal{E} = \mathcal{E}^*/10 \) locates the regime for which the variation of the PEDM is discussed in the text.

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