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Dipolar collisions of ultracold polar molecules in a microwave field

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Collisions at ultracold temperatures between $^1\Sigma$-state diatomic polar molecules in a circularly polarized microwave field are theoretically analyzed. We demonstrate that elastic and inelastic collisions of polar molecules at ultracold temperatures are affected by an external microwave field and that they are enhanced at resonance frequencies. We show that the collision dynamics of polar molecules in a microwave field is largely determined by the long-range dipole-dipole interaction. Through this interaction, two polar molecules can resonantly exchange internal energy by undergoing a transition between neighboring rotational levels. This process may stabilize the system and enable the successive evaporative cooling of molecules. This paper discusses fermionic polar molecules at ultralow temperatures (1 μK).

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I. INTRODUCTION

Recent progress in creating and manipulating ultracold polar diatomic molecules [1–13] has inspired the exploration of new methods for achieving quantum control and manipulating collisions. Because of its rotational nature, a microwave field can be used to manipulate the states of ultracold polar diatomic molecules. Molecular motion and interactions between molecules can be controlled through both the amplitude and the frequency of microwave radiation. There are other relatively well-established methods for controlling cold atoms, such as Feshbach resonance and optical shielding. However, polar molecules at low energies exhibit several distinctive characteristics. First, a large dipole moment permits the manipulation of strongly correlated condensed-matter-like systems [14–24], two-body interactions [25–37], and three-body interactions [38]. Second, a combination of static and dynamic electric fields can be used to enhance elastic collision rates and suppress inelastic ones in a more sophisticated way than other techniques [39]. Third, the spontaneous-emission lifetimes of rotational states are much longer than typical trap times, making it possible to design microwave traps that are much larger than optical traps [40]. This makes it possible to use very small detunings and so investigate different regimes using microwave fields with low to high electric fields and low to high frequencies. Thus, microwave traps can potentially be large and deep and have the ability to trap many molecules at temperatures as high as 1 K. However, collisional cooling (evaporative or sympathetic) seems to be the only way to achieve ultracold temperatures and sustain dense samples. In a previous study [26], we considered various aspects of the collision dynamics of cold polar molecules in a circularly polarized microwave field. We considered dipolar collisions and sought to determine how to control them using a microwave field. The use of microwave fields to control collisions between cold polar molecules and atoms has been analyzed [41–43] and it has been demonstrated that microwave fields induce couplings between Zeeman states and thus enhance inelastic relaxation. It has also been demonstrated that Feshbach resonances can be tuned by varying both the intensity and the frequency of the microwave field. Microwave fields have been shown to have the same effect on Feshbach resonances for NH-NH collisions [43] for which the long-range dipole-dipole interaction may be more influential. The main difference between molecule-molecule and molecule-atom systems is that applying an electric field to two polar molecules induces a strong long-range dipole-dipole interaction, whereas a molecule and an atom interact only through short-range interactions. Consequently, applying an ac electric field to a molecule-molecule system can generate larger and deeper traps than for molecule-atom systems. Another important aspect of molecule-molecule systems is that they can undergo chemical reactions even at ultracold temperatures [44–47]. Some of them, such as alkali-metal dimers KRb and LiCs, have exergonic reactive collision channels [48] even when they are in their vibrational and rotational ground state. Moreover, the reaction-rate constant increases with increasing electric-field strength as the dipole-dipole interaction is activated [49]. Some other bialkali molecules (e.g., RbCs) have no reactive channels in their rovibrational ground state and are thus promising for obtaining stable molecular systems in the quantum regime. Accounting for chemical reactions is beyond the scope of the present study and thus our analysis of dipolar collisions in a microwave field is only appropriate for molecules with no reactive channels in their ground state. In the present study, we investigate dipolar collisions of $^1\Sigma$ polar molecules in their rotational and vibrational ground state trapped in a circularly polarized microwave field. We consider circular polarization rather than linear polarization since ac-Stark shifts contain many avoided crossings, which enhance the collisional loss [40]. We consider low-temperature collisions of polar molecules in the strong molecule-field coupling and strong resonant molecule-field coupling regimes. As polar molecules have large permanent electric dipole moments, the strong dipole-dipole interaction can be activated in such regimes and thus the collision dynamics in a relatively strong external microwave field is mostly determined by this long-range, anisotropic interaction:

$$V_{DD}(\mathbf{R},\omega_{\mathbf{A}},\omega_{\mathbf{B}}) = \frac{\mu_1 \cdot \mu_2 - 3(\hat{\mathbf{R}}\cdot\mu_1)(\hat{\mathbf{R}}\cdot\mu_2)}{R^3}$$
$$= -\frac{\sqrt{6}}{R^3}\sum_q (-1)^q C^2_{-q}(\omega)[\mu_1\otimes\mu_2]^2_q, \quad (1)$$

where $\omega_{A,B} = (\theta_{A,B},\phi_{A,B})$ are the polar angles of molecules A and B with respect to the laboratory-fixed quantization axis and $\mathbf{R} = (R,\omega)$ is the vector connecting the centers of mass of the molecules in the laboratory-fixed coordinate frame. Here, $C^2_{-q}(\omega)$ is a reduced spherical harmonic. The short-range potential for the diatom-diatom interaction is generally unknown or poorly known. It is not generally possible to completely ignore the short-range interaction, even when the collision dynamics is mostly determined by the dipole-dipole interaction. However, collisions of ultracold (i.e., temperatures below $E_D = \mu^2_{\rm eff}/D^3$) polar molecules in their ground state possess a universal threshold under a wide variety of circumstances [29, 37]; in other words, threshold cross sections approach the Born limit of $\sigma \propto D^2$, where $D = M\mu^2_{\rm eff}/\hbar^2$ is the dipole length, M is the reduced mass, and $\mu_{\rm eff}$ is the effective electric dipole moment. This universality does not hold for bosonic species at resonances where threshold cross sections are determined by the s-wave scattering length [29]. Due to the strong dipole-dipole interaction, the dipole length D is the dominant factor and it is much larger than the size scale (typically R_0–100 a.u.) below which short-range interactions become significant. For example, short-range boundaries for KRb and RbCs molecules lie between 50 and 80 a.u., which are shorter than the van der Waals length [50]. Because the present study considers ultracold molecules, the discussion can be simplified by replacing the short-range interaction by a zero boundary condition for the wave function at a fixed interparticle separation of $R_0 \ll D$. This approximation is not helpful when it is desired to describe resonances precisely, which requires an exact knowledge of the short-range potentials. The strong long-range dipole-dipole interaction between ground-state polar molecules can be activated by both dc and ac fields. The advantages of ac fields have been briefly described by DeMille [40]. The main disadvantage of using ac fields is that even ground-state molecules may undergo inelastic collisions, resulting in collisional losses. Here, inelastic processes refer to processes in which spin changing transitions occur that do not involve other losses, such as those due to chemical reactions. We thus wish to determine how critical this disadvantage is and whether polar molecules can survive collision-induced Stark relaxation processes and so be used for evaporative cooling in microwave traps.

We expect to find the same universal threshold behavior that has previously been observed [29,37], but the dipole length and the effective dipole moment depend on both the electric-field strength and the microwave frequency. On the whole, collisions at ultracold temperatures are mostly controlled by the two ratios ν/B and $\mu\mathcal{E}/hB$, where ν is the microwave frequency, B is the molecular rotational constant, and $\mathcal{E}$ is the electric-field strength. As we show below, this is also true for inelastic collisions of polar molecules and such collisions are very sensitive to these two parameters. This phenomenon can be clearly explained in terms of the field-dressed formalism, which is a very appropriate approach for studying slow collisions in ac fields because molecules can essentially be "dressed" by such fields. As a dressed state is a superposition of many pure states, inelastic collisions always occur between dressed molecules (although they may have small cross sections) and inelastic collisions can be drastically enhanced in strong and/or resonant fields. The main reason why collisions are inelastic is that dressed molecules effectively interact through the dipole-dipole potential, whereas a larger field in conjunction with a smaller detuning produces a stronger dipole-dipole interaction. In the present case, we consider polar molecules to be rigid rotors so that a dressed state is a superposition of rotational states $|J,M_J\rangle$. We are interested in collisions of polar molecules in the dressed state, which evolves adiabatically from the absolute ground state at zero field, $|J=0,M_J=0\rangle$. This dressed state is a superposition of $|0,0\rangle$, $|1,\pm 1\rangle$, $|2,\pm 2\rangle,\ldots$ states in the circularly polarized microwave field. If the microwave frequency is considerably smaller than the energy of the first excited rotational state (i.e., $\nu \ll 2B$), then few two-body inelastic collisions will occur so that collision losses will be small. This condition will be satisfied when there is a weak field ($\mu\mathcal{E} \ll hB$). In this case, almost no inelastic collisions will occur, as almost all of the molecules will be in the pure $|0,0\rangle$ state, which is beneficial for evaporative cooling. However, we are not currently interested in this case because at such weak fields the dipole-dipole interaction will not be strongly activated, as the effective dipole moment will be very small. Thus, it is not a long-range interaction system. We require a larger field to exploit dipoles and small detunings (near-resonance frequencies) to obtain a greater trap depth, which implies $\nu \sim B$ and $\mu\mathcal{E} \sim hB$. However, an unfortunate consequence of such field parameters is that inelastic collisions are enhanced under such conditions and molecules are already essentially dressed by a microwave field and so undergo many more inelastic collisions [26]. We analyze the nature of such inelasticity and define the range of parameters for which the system will have long interactions and have reasonably small inelastic rates. We show that it is possible to have relatively small inelastic cross sections at different nonresonance frequencies such as $2B < \nu < 4B$, where $2B, 4B, \ldots$ are resonance frequencies if the field strength is relatively large (i.e., $\mu\mathcal{E} \sim hB$). Here resonance frequencies correspond to the energy differences between the neighboring rotational states.

Collisions in external fields not only enhance inelastic processes, but also affect elastic processes. The latter is rather well known and has been studied for many cases [29,37, 43,51,52]. However, elastic processes in a microwave field have their own peculiarities, which can be better understood in the field-dressed molecule picture. We found that at large fields (i.e., $\mu\mathcal{E} > hB$), the dipolar elastic collisions (elastic collisions which are mostly determined by the dipole-dipole interaction; see Sec. III) dominate over other collisions and may provide successive evaporative cooling, especially for fermionic molecules. The main aim of this study is to determine the collision dynamics of ultracold polar molecules in a microwave field. At ultracold temperatures, the long-range dipole-dipole interaction follows the general behavior of a molecule-molecule scattering process and it is sensitive to the parameters of an external microwave field. In this study, we focus on collisions of polar molecules in their strong-field-seeking state; in other words, polar molecules prepared in the absolute ground state and irradiated by a microwave field. After discussing the model properties of $^1\Sigma$ molecules in Sec. II, we consider and illustrate some field-dependent characteristics of elastic and inelastic cross sections in Sec. III.

II. MODEL

The dressed-state formalism is particularly convenient for describing the photon-atom interaction in the strong-field limit [53,54], where the dressed states are eigenstates of the Hamiltonian of the total system: particle plus photon. The same holds for the molecule-field interaction. The idea of using the field-dressed formalism for low-temperature atomic collisions in optical traps was proposed and analyzed in [55–58]. Using the basic ideas of this approach, we adapted it to analyze the collisional dynamics of cold polar molecules in a microwave cavity. To simulate dipolar collisions, we choose "typical" (for heteronuclear alkali-metal dimers [59]) dipole moment $\mu = 1$ D.

A. Polar $^1\Sigma$-type molecules in a circularly polarized microwave field

Here we analyze the ac-Stark effect for a polar molecule in a circularly polarized microwave field and build dressed states which are used for quantum scattering calculations. The energy levels of $^1\Sigma$-type molecules can be described by rotation J, total spin F (i.e., including nuclear spin), and vibration υ quantum numbers. To simplify things, we will neglect hyperfine splitting and consider molecules only in the $\upsilon = 0$ vibrational ground state. So we treat polar molecules as rigid rotors with a permanent dipole moment. The basis states of the rigid rotor plus field Hamiltonian $H = H_{\rm rot} + H_{\rm field}$ are

$$|J,M,n\rangle \equiv |JM\rangle|\bar{N}+n\rangle, \tag{2}$$

where M is the projection of J on the space-fixed axis, which is conveniently chosen parallel to the wave vector of the microwave field, $\bar{N}+n$ is the dressed-state photon number, and $n \ll \bar{N}$ is the deviation of the photon number. The ac-Stark splitting is caused by the molecule-field interaction $H_{\rm Stark} = -\vec{\mu}\vec{\mathcal{E}}$. Thus the energy levels of the molecule in the microwave field can be found by diagonalizing the following Hamiltonian in the basis set (2) [60]:

$$\begin{aligned} H_{{\rm mol},f} &= H_{\rm rot} + H_{\rm field} + H_{\rm Stark} \\ &\equiv B_e\hat{J}^2 + h\nu(a^\dagger a - \bar{N}) - \frac{\mu\mathcal{E}}{2}\frac{1}{\sqrt{\bar{N}}}[(\mathbf{n}\cdot\epsilon^*)a^\dagger \\ &\quad + (\mathbf{n}\cdot\epsilon)a]. \end{aligned} \tag{3}$$

Considering the circularly polarized microwave field (σ^-), the nonzero Hamiltonian matrix elements (normalized by hB) are given by [40]

$$\langle J,M,n|H_{\rm rot} + H_{\rm field}|J,M,n\rangle = J(J+1) + n\frac{\nu}{B}, \tag{4}$$

$$\begin{aligned} &\langle J+1,M+1,n+1|H_{\rm Stark}|J,M,n\rangle \\ &\quad = \frac{x}{2}\frac{\sqrt{J+M+1}\sqrt{J+M+2}}{\sqrt{2J+1}\sqrt{2J+3}}, \\ &\langle J-1,M-1,n-1|H_{\rm Stark}|J,M,n\rangle \\ &\quad = \frac{x}{2}\frac{\sqrt{J-M+1}\sqrt{J-M+2}}{\sqrt{2J+1}\sqrt{2J+3}}, \end{aligned} \tag{5}$$

where $x = \mu\mathcal{E}/hB$. Here, it is assumed that n is much smaller than the mean photon number $\bar{N}$. In the case of the circularly polarized field, which can be seen from the above matrix elements [Eq. (4)], absorption (emission) of a photon is accompanied by a change in angular momentum projection M by 1. Figure 1 shows the energies of dressed states versus applied electric-field frequency for the $J = 0$ and $J = 1$ states at $x = 0.3$ within the $\nu/B = [0,4]$ frequency range and versus the applied ac-field strengths at some frequencies. The ac-Stark shifts determine the trap depths for different states as well. It should be noted that we show [Figs. 1(b)–1(d)] dressed states $|\widetilde{(JMn)}\rangle$ with different numbers of photons, which can be seen as a repetitive bunch of curves.

The dressed states of trapped molecules are not pure states but the superposition of many states (see Sec. II B). Only at weak fields ($x \ll 1$) and far-from-resonance frequencies are molecules mostly in one state. For example, the dressed "ground state" (it is marked as $|000\rangle$) molecules are mostly in the $J = 0, M = 0$ state at $\nu < 2B$ frequencies, in the $J = 1, M = -1$ state at $2B < \nu < 4B$, in the $J = 2, M = -2$ state at $4B < \nu < 6B$, and so on [Fig. 1(a)]. At around the resonance frequency $\nu = 2B$, our state is a 50/50 superposition of the $J = 0, M = 0$ and the $J = 1, M = -1$ states, while at around the resonance frequency $\nu = 4B$, our state is a 50/50 superposition of the $J = 1, M = -1$ and the $J = 2, M = -2$ states, and so on. At strong fields ($x \gg 1$), a dressed state will be a superposition of many states, even far-from-resonance frequencies.

The trap depth is defined by both the strength of a microwave field and its frequency, while the frequency determines if molecules at a given state are attracted to or repelled out of the region of a strong microwave electric field. For example, if one wants to trap (attract) ground-state ($J = 0, M = 0$) molecules to regions of a strong field, then the detuning $\Delta = \nu - 2B$ from the $J = 0 \leftrightarrow J = 1$ resonance must be smaller than zero [Figs. 1(a) and 1(b)]. For the positive detuning, the depth for $J = 1, M = -1$ state molecules will be the largest, while ground-state molecules will be mostly repelled out of it [Figs. 1(a) and 1(c)]. It should be noted that the dressed $|000\rangle$ state is mostly the $J = 1, M = -1$ state for positive detunings at weak fields ($x \ll 1$) and far-from-resonance frequencies. The same is applied for order resonance frequencies: if the detuning $\Delta = \nu - 4B$ from the $J = 1 \leftrightarrow J = 2$ resonance becomes positive, then molecules in $J = 2, -2$ states will be mostly attracted to a strong-field region, while molecules in $J = 1$ and $J = 0, M = 0$ states will be mostly repelled out of it and the depth for the $J = 2, M = -2$ state will be the largest [Fig. 1(d)].

B. Dressed states

The ac-electric field mixes states with different J, M, and n and hence neither of them is a good quantum number. Thus we can only mark our states by their origin at zero field (Fig. 1), where they can be assigned by J and M quantum numbers.

In practice, we transform the molecular state to a field-dressed basis for performing scattering calculations, and the state with a given mean photon number $\bar{N}$ is described as

$$|\widetilde{(JMn)}\rangle \equiv |\widetilde{(JMn)};\vec{\mathcal{E}}\rangle = \sum_{JMn} p_{(JMn)}|JMn\rangle, \tag{6}$$

where $p_{(JMn)}$ stands for the eigenfunctions of the $H_{{\rm mol},f}$ Hamiltonian (3) determined numerically at each value of the field. We will continue to refer to the molecular states by the

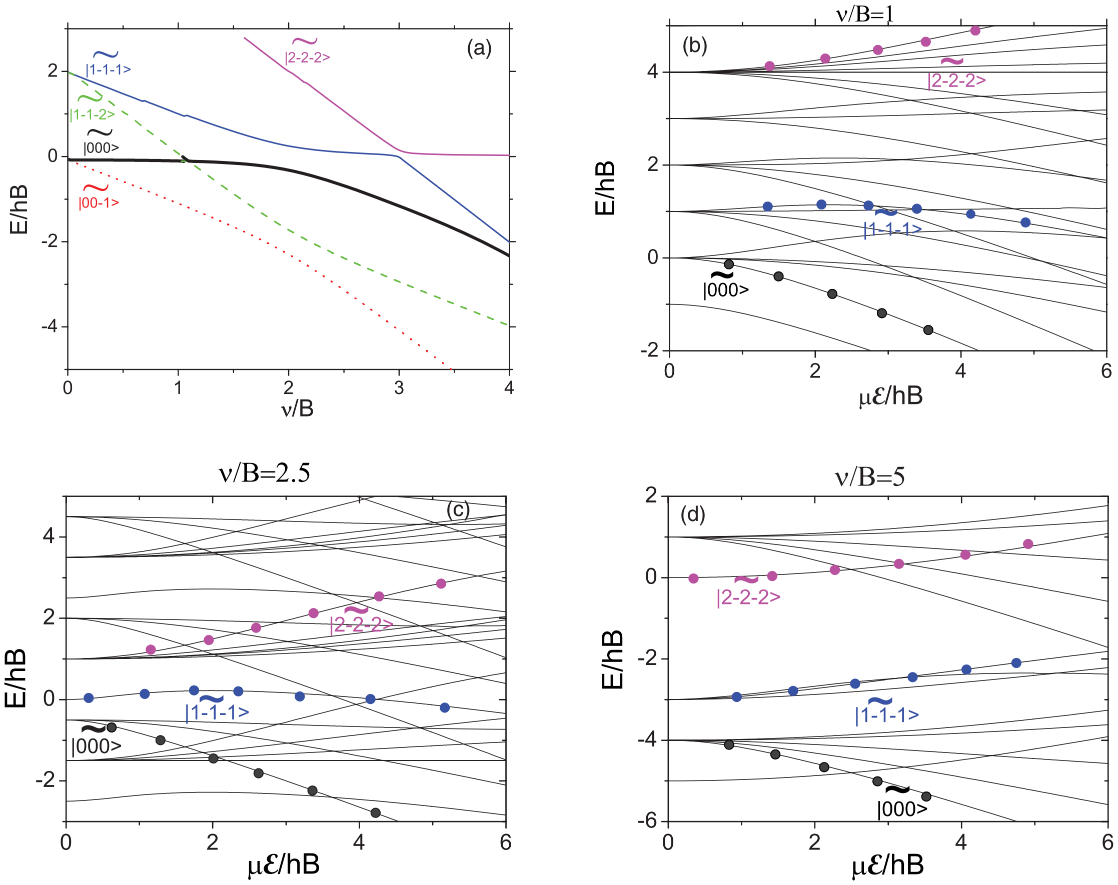

FIG. 1. (Color online) (a) The energies of dressed states vs the applied ac-field frequency at $\mu E/hB = 0.3$. (b)–(d) The energies of dressed states vs the applied ac-field strengths.

quantum numbers J, M, and n, with the understanding that they are only approximately good in a field, and that Eq. (6) is the appropriate molecular state. Note that ac-Stark splitting should be irrelevant to the value of $|n|$ as $n \ll \bar{N}$, so we choose small values of n. For the numerical calculations, the Hilbert space should be truncated at some values of J and n. The larger the field, the larger values of J and n should be taken into account simultaneously. As we are not going to consider cases with a very large field ($x \gg 1$), we truncate the Hilbert space by $J_{\max} = 2$ and $-1 \leqslant n \leqslant 1$ values. Figure 2 shows the dressed-state energy-level diagram for the rotational states of a diatomic molecule in a circularly polarized microwave field for such a truncation. The ac-Stark splitting is the same for each manifold, $\bar{N}+0$, $\bar{N}-1$, or $\bar{N}+1$, as states from different manifolds are not connected and the energies of neighboring manifolds are simply shifted on the $h\nu$ energy [Figs. 1(b)–1(d)]. But the dipole-dipole interaction can cause transitions between the neighboring manifolds (orange arrows on Fig. 2). The $\bar{N}+0$ manifold consists of three states: $|000\rangle$, $|1-1-1\rangle$, and $|2-2-2\rangle$. Then we will mark the states for this manifold as $|\widetilde{000}\rangle$, $|1-\widetilde{1}-1\rangle$, and $|2-\widetilde{2}-2\rangle$. The same marking stands for other manifolds.

III. DIPOLAR COLLISIONS IN A MICROWAVE FIELD

Collisional dynamics in a microwave field has it own peculiarities, which can be better understood in the field-dressed molecule picture. For example, let us consider collisions of two-level molecules in a circularly polarized (σ^-) microwave field for the case when the levels are the ground state $J=0$ and the first excited rotational state $J=1$. As we are considering a σ^- polarized field, we only need to consider the $|J=1, M_J=-1\rangle$ state. Following [53,60], the molecule-field interaction couples these two unperturbed

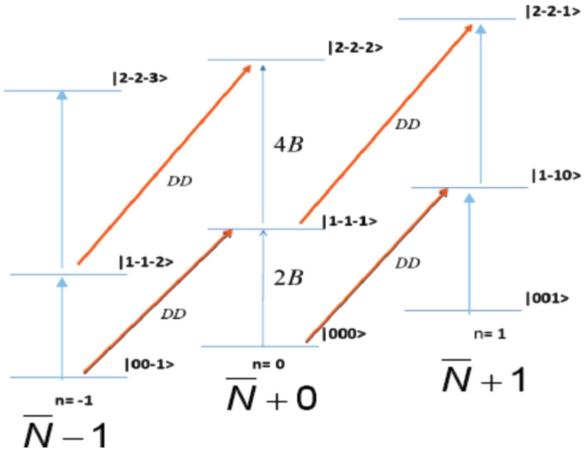

FIG. 2. (Color online) The dressed-state energy-level diagram for the rotational states of a diatomic molecule in a circularly polarized microwave field. The $\bar{N}+0$ and $\bar{N}\pm 1$ manifolds are shown.

states, $|J=0,M_J=0\rangle|\bar{N}\rangle$ and $|J=1,M_J=-1\rangle|\bar{N}-1\rangle$, and we obtain two perturbed or dressed states,

$$\begin{aligned}|1(\bar{N})\rangle &= \cos\theta|J=0,M_J=0\rangle|\bar{N}\rangle\\ &\quad+\sin\theta|J=1,M_J=-1\rangle|\bar{N}-1\rangle,\\ |2(\bar{N})\rangle &= -\sin\theta|J=0,M_J=0\rangle|\bar{N}\rangle\\ &\quad+\cos\theta|J=1,M_J=-1\rangle|\bar{N}-1\rangle,\end{aligned} \tag{7}$$

where $|\bar{N}+n\rangle$ are the photon number states, $\bar{N}$ is the average number of photons in the field mode, and $\tan 2\theta=-\Omega/\Delta$, where Ω is the Rabi frequency. If we consider collisions of two molecules in the dressed $|1(\bar{N})\rangle$ state, then we can formally state that if both molecules remain in the same $|1(\bar{N})\rangle$ state after scattering, then the process is elastic: $|1(\bar{N})\rangle_1|1(\bar{N})\rangle_2 \Longrightarrow |1(\bar{N})\rangle_1|1(\bar{N})\rangle_2$. However, this is not the only possible elastic process in our formalism and this definition of elastic collisions excludes another important elastic process. As our dressed states are a superposition of the $|J=0,M_J=0\rangle|\bar{N}\rangle$ and $|J=1,M_J=-1\rangle|\bar{N}-1\rangle$ states, elastic scattering of these unperturbed states implies that only two elastic processes, $|0,0\rangle_1|0,0\rangle_2 \Longrightarrow |0,0\rangle_1|0,0\rangle_2\rangle$ and $|1,-1\rangle_1|1,-1\rangle_2 \Longrightarrow |1,-1\rangle_1|1,-1\rangle_2$, are possible because a two-body interaction does not alter the number of photons (since the number of photons are conserved for two-body matrix elements). On the other hand, the process $|1(\bar{N})\rangle_1|1(\bar{N})\rangle_2 \Longrightarrow |1(\bar{N})-1\rangle_1|1(\bar{N})+1\rangle_2$ is also elastic because both the incident and final channels have almost the same energies in the strong-field limit $\bar{N}\gg 1$. In terms of our unperturbed states, such elastic scattering is simply the $|0,0\rangle_1|1,-1\rangle_2 \Longrightarrow |1,-1\rangle_1|0,0\rangle_2\rangle$ process. Formally, this process implies that two polar molecules resonantly exchange internal energy by undergoing a transition between the $|J=0,M=0\rangle$ and $|J=1,M=-1\rangle$ levels. In the present case, this can only occur by the dipole-dipole interaction, as the matrix element for the direct term is zero. This classification of elastic collisions into two types assists in analyzing the role of the dipole-dipole interaction. Namely, the latter elastic collisions are mostly determined by the dipole-dipole interaction, whereas the same is not true for the former elastic collisions (since the diagonal matrix elements for the dipole-dipole interaction are absent). We refer to such collisions as dipolar elastic collisions. However, it is important to remember that the dipole-dipole interaction is also involved, although to a lesser degree, in the first elastic process.

A. Scattering formalism

Here, diatomic molecule-diatomic molecule scattering in the presence of a microwave field is modeled in terms of the interactions between two rigid rotors with permanent dipole moments. Our model only accounts for dipole-dipole interactions, which provide the largest contribution to the collisional dynamics. In practice, prior to each scattering calculation, we numerically transform the molecular state to a field-dressed basis defined by (2). The coupled-channel Schrödinger equations in the field-dressed basis take the usual form,

$$\left\{\frac{d^2}{dR^2}\mathbf{I}+\frac{2m}{h^2}[E\mathbf{I}-\mathbf{E}_{\mathbf{th}}(\mathcal{E},\nu)-\mathbf{V}(R,\mathcal{E},\nu)]\right\}\tilde{\mathbf{F}}(R,\mathcal{E},\nu)=0, \tag{8}$$

where $\mathcal{E}$ is the magnitude and ν is the frequency of the microwave field used to parameterize these equations, $\mathbf{E}_{\mathbf{th}}(\mathcal{E},\nu)$ is the diagonal matrix of the threshold energies (i.e., the Stark energies),

$$\begin{aligned}\mathbf{V}(R,\mathcal{E},\nu) \Rightarrow{}& \langle\beta_1|\otimes\langle\beta_2|\otimes\langle lM_l|V(\omega_A,\omega_B,\omega,R)|\beta_1'\rangle\otimes|\beta_2'\rangle\\ &\otimes|l'M_l'\rangle\end{aligned} \tag{9}$$

is the matrix containing the dipole-dipole interactions and the centrifugal potential, and $\tilde{\mathbf{F}}(R,\mathcal{E},\nu)$ is the matrix of radial wave functions in the field-dressed basis,

$$\tilde{\Psi}^{\mathcal{M}_c}=\sum_{\beta_1,\beta_2,l,M_l}\{|\beta_1\rangle\otimes|\beta_2\rangle\otimes|lM_l\rangle\}^{\mathcal{M}_c}\tilde{\mathbf{F}}^{\beta_1,\beta_2,\mathcal{M}_c}(R,\mathcal{E},\nu), \tag{10}$$

where $\{\cdot\}^{\mathcal{M}_c}$ is the angular part of this wave function, $|\beta\rangle\equiv|(\widetilde{JMn})\rangle$ is the wave function for each molecule, and M_l is the projection of the partial-wave quantum number l on the laboratory axis. As an external microwave field is circularly polarized (σ^-), the $z$component of the total angular momentum of the system of two molecules plus field, $\mathcal{M}_c=(M_1+M_2+m_l-N)\hbar$, is conserved, where each of N photons has an angular moment $-\hbar$ [60]. In practice, we use $\mathcal{M}_c=(M_1+M_2+m_l-n)\hbar$, where n is a deviation of the photon number from the mean photon number $\bar{N}$. Thus we express our Hamiltonian in a basis of total angular momentum $\mathcal{M}_c$. Since the projection of total angular momentum of the system on the field axis, $\mathcal{M}_c$, is a conserved quantity, calculations can be performed for each value of $\mathcal{M}_c$ separately. We generally find that the dominant contribution to cross sections arises from the minimal allowed absolute value of $\mathcal{M}_c$ and that the general behavior of cross sections for another $\mathcal{M}_c$ is quite similar, and so we restrict calculations accordingly.

We solve these equations using the logarithmic-derivative propagator method [61] to determine the scattering matrices. These matrices are then used to calculate the total state-to-state cross sections according to the procedure described in [62].

B. Microwave field dependence

The channel states of the scattering problem under consideration are

$$|\beta_1\rangle\otimes|\beta_2>\otimes|lM_l\rangle\equiv|(\widetilde{JMn}),(\widetilde{JMn})'\rangle\otimes|lM_l\rangle. \tag{11}$$

Because collisions between two identical particles are considered here, it is necessary to introduce a symmetrized basis:

$$\begin{aligned}&\{|\beta_1\rangle\otimes|\beta_2\rangle\otimes|lM_l\rangle\}_{\mathrm{sym}}\\ &\quad=\frac{[|\beta_1\rangle\otimes|\beta_2\rangle+\eta(-1)^l|\beta_2\rangle\otimes|\beta_1\rangle]\otimes|lM_l\rangle}{[2(1+\delta_{\beta_1\beta_2})]^{1/2}},\end{aligned} \tag{12}$$

where η accounts for the exchange symmetry. For fermionic molecules at ultralow temperatures, for most cases it is sufficient to account only for the p-wave ($l=1$) and f-wave ($l=3$) partial waves. We are particularly interested in the lowest-energy strong-field-seeking state for the $N+0$ manifold. This $|(\widetilde{000})\rangle$ state is indicated by the black circles in Fig. 1. As mentioned in Sec. II A, the energy levels for each manifold are the same as those of the ac-Stark shifts. As such, it is sufficient to consider molecules in their incident channels from any manifold, and the $N+0$ manifold is the most convenient. Dipole-dipole interactions can induce transitions between different manifolds, which can produce inelastic relaxation. For example, the inelastic channels for our incident channel $|(\widetilde{000}),(\widetilde{000})\rangle$ are

$$|(\widetilde{00-1}),(\widetilde{00-1})\rangle,|(\widetilde{00-1}),(\widetilde{1-1-2})\rangle,\\ |(\widetilde{1-1-2}),(\widetilde{1-1-2})\rangle, \tag{13}$$

$$|(\widetilde{00-1}),(\widetilde{2-2-3})\rangle,|(\widetilde{1-1-2}),(\widetilde{2-2-3})\rangle,\\ |(\widetilde{2-2-3}),(\widetilde{2-2-3})\rangle, \tag{14}$$

and so on. Larger frequencies and field strengths result in larger contributions of the channels to the total inelastic cross section. It should be noted that all final states of an inelastic process belong to the $N-1$ manifold for both molecules. The states of the $N-2$ manifold only provide second-order contributions to the total inelastic cross section and can be safely neglected here. The threshold energies of the channels of the $N+1$ manifold are higher than the threshold energy of our incident channel and do not contribute significantly to the scattering dynamics at ultracold temperatures. However, in contrast to the inelastic channels defined above, the $|(\widetilde{00-1}),(\widetilde{001})\rangle$ channel states belong to different manifolds: the $|(\widetilde{00-1})\rangle$ state belongs to the $N-1$ manifold, whereas the $|(\widetilde{001})\rangle$ state belongs to $N+1$ manifold. Additionally, the threshold energies of this channel and our incident channel are equal in the limit of a strong field ($N \rightarrow \infty$). Another important feature is that to a first-order approximation, these two channels interact strictly through dipole-dipole interactions:

$$\langle(\widetilde{000}),(\widetilde{000})|V_{DD}|(\widetilde{00-1}),(\widetilde{001})\rangle\\ \propto \langle(00),(1-1)|V_{DD}|(1-1),(00)\rangle. \tag{15}$$

Thus, the $|(\widetilde{000}),(\widetilde{000})\rangle \Longrightarrow |(\widetilde{00-1}),(\widetilde{001})\rangle$ process is caused, to the first-order approximation, by the exchange of ground $|J=0,M_J=0\rangle$ and excited $|J=1,M_J=-1\rangle$ rotational states, and it is isoenergetic. Formally, this exchange describes dipolar elastic collisions and is the process described above. The elastic $|(\widetilde{000}),(\widetilde{000})\rangle \Longrightarrow |(\widetilde{000}),(\widetilde{000})\rangle$ process, to the first order, can only proceed through short-range interactions.

Figure 3 shows the total elastic and total inelastic cross sections at cold temperatures for our prototype molecule. Here the total elastic cross section is the sum of cross sections for the $|(\widetilde{000}),(\widetilde{000})\rangle \Longrightarrow |(\widetilde{00-1}),(\widetilde{001})\rangle$ process, which we called the dipolar elastic one, and the $|(\widetilde{000}),(\widetilde{000})\rangle \Longrightarrow |(\widetilde{000}),(\widetilde{000})\rangle$ process, which is the "ordinary" elastic one. For our initial state $|(\widetilde{000}),(\widetilde{000})\rangle$, channels with $\mathcal{M}_c = 0, \pm 1$ give the main contribution, as only they have contributions from the p-wave scattering. At ultracold temperatures, contributions from larger $|\mathcal{M}_c|$ become large at larger fields ($x \gtrsim 1$) and/or near resonance frequencies ($\nu/B = 2,4,\ldots$). Figure 3 shows a typical behavior of cross sections near and far from resonance frequencies at a rather small field strength ($x = 0.01$). The case in which the resonance frequency is $\nu/B = 2$ is shown in Fig. 3(a). At this frequency, the dipolar elastic process is dominant, and at a temperature below ~1 μK the total elastic cross section follows the well-known Wigner threshold law for dipolar collisions, $\sigma_{\text{dip}} \propto$ const, as a consequence of the fact that the dipole-dipole interaction is fully engaged. In the case of a far-from-resonance field [Fig. 3(b)], the dipole-dipole interaction is weak and the elastic cross section follows the Wigner threshold law for short-range interactions, namely, $\sigma_{el} \propto E^2$. The inelastic cross sections at threshold regime obey the familiar Wigner law for p waves, $\sigma_{\text{in}} \propto E^{1/2}$, at any frequency. One can see that the inelastic cross sections are quite large for ground-state molecules at the resonance frequency, as both elastic and inelastic processes are enhanced by the strong dipole-dipole interaction.

Figure 4 shows contributions from different channels to the total cross sections only for the $\mathcal{M}_c = 1$ case. It is clearly seen that with changing field frequency, from its resonance value ($\nu/B = 2$) through some intermediate value ($\nu/B = 1.5$) to the far-from-resonance case ($\nu/B = 1$), the threshold behavior for the elastic process becomes less and less of the dipolar nature and eventually follows the Wigner law for short-range interactions. As we noted above, the cross section of dipolar elastic collisions rather precisely follows universal, $\sigma_{\text{dip}} \propto D^2$, threshold behavior, while the threshold behavior of elastic collisions follows the well-known formula for the p-wave scattering of two indistinguishable fermions [63], $\sigma_{el} = 24\pi k^4 a_p^2$, where k is a wave number and a_p is a scattering volume. As we do not have a realistic short-range potential, here it is defined by the effective van der Waals forces C_6/R^6, where $C_6 = \mu_{\text{eff}}^4/4B$. In this case, the scattering volume can be estimated by the simple semiclassical formula [64] $a_p = \bar{a}_p[1 + \tan(A -$

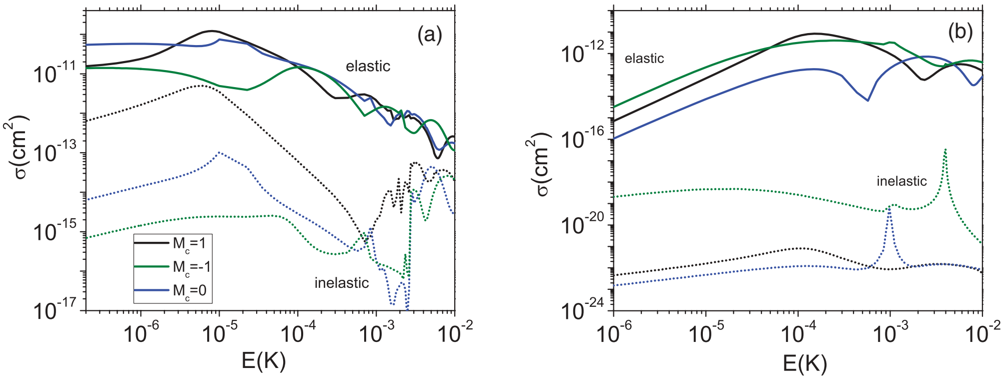

FIG. 3. (Color online) Total elastic (solid lines) and total inelastic (dotted lines) cross sections vs the collisional energy for (a) $\nu/B = 2$ and (b) $\nu/B = 1$ at $x \approx 0.01$ strength for the prototype molecule with $\mu = 1$ D. See the text for details.

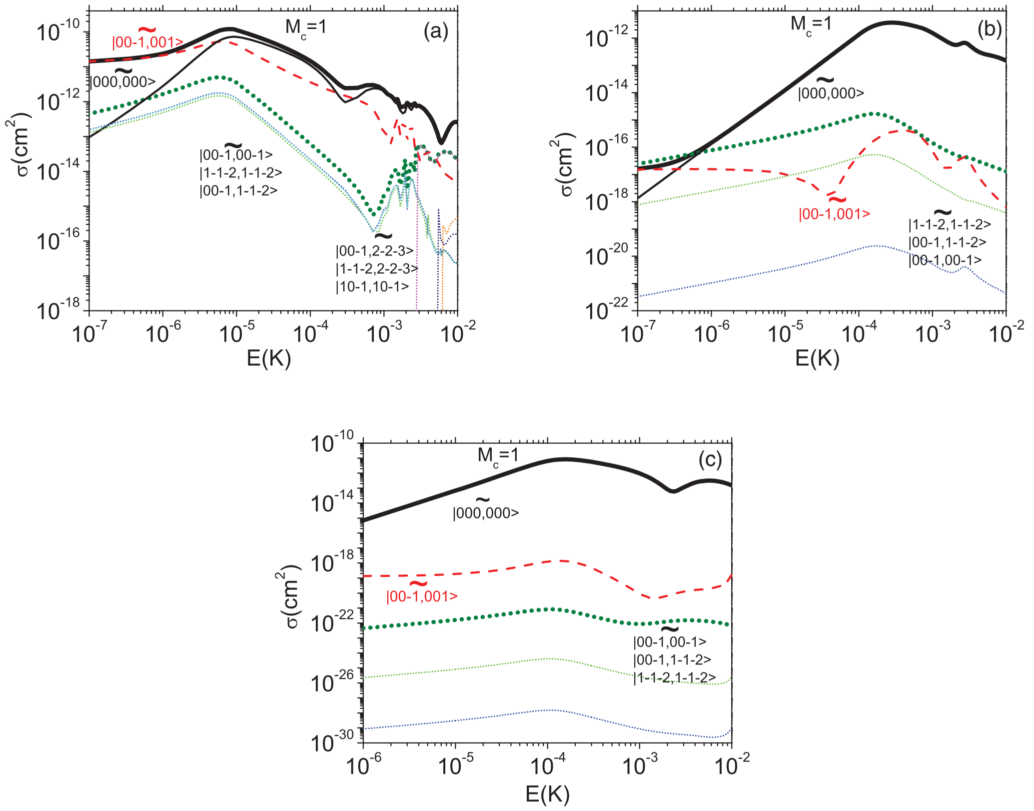

FIG. 4. (Color online) Total elastic (thick solid lines), elastic (solid lines), dipolar elastic (dashed lines), and total inelastic (thick dotted lines) cross sections vs the collisional energy for (a) $\nu/B \approx 2$, (b) $\nu/B = 1.5$, and (c) $\nu/B = 1$ at $x \approx 0.01$ strength for the prototype molecule with $\mu = 1$ D. State-to-state inelastic cross sections are shown by thin lines of a different color. See the text for details.

$3\pi/8)]$, where $\bar{a_p} = (2mC_6/\hbar^2)^{3/4}\Gamma(1/4)/[24\sqrt{2}\Gamma(7/4)]$ and $A = (1/\hbar)\int_{R_-}^{\infty}\sqrt{-2mV(R)}dR$. This means that the "typical" elastic cross section can be described reasonably well, knowing only the mean scattering volume $\bar{a_p}$ in the case that is far from a p-wave resonance, which means that the typical elastic cross section is mostly defined by the dipole moment and the rotational constant. It is quite easy to verify that as soon as the van der Waals length $l_{vdW} = (2mC_6/\hbar^2)^{1/4}$ becomes larger than the dipole length D, the threshold behavior mostly follows the Wigner law for short-range interactions [Figs. 4(b) and 4(c)]. Although, if both of these lengths are of the same order, one can find a transition from $\sigma_{\text{tot}.el} \propto E^2$ to $\sigma_{\text{tot}.el} \propto D^2$ behavior [Fig. 4(b)] at ultracold temperatures.

The main contribution to the total inelastic cross section comes from the relaxation to the $|(\widetilde{00-1}),(\widetilde{00-1})\rangle$ channel, which is true at least for frequencies smaller than the first resonance one ($\nu/B = 2$). But for near-resonance frequencies [Fig. 4(a)], the other inelastic cross sections are rather large as well, and considerable contributions from other channels $[|(\widetilde{00-1}),(\widetilde{2-2-3})\rangle, |(\widetilde{1-1-2}),(\widetilde{2-2-3})\rangle, |(\widetilde{10-1}),(\widetilde{10-1})\rangle]$ appear at lower temperatures when these channels become open. Here we would like to mention the peculiarity of the $|(\widetilde{00-1}),(\widetilde{00-1})\rangle$ state noted in [26], namely, that the relaxation to this channel cannot cause any trap losses, as both molecules do not change their internal states but only transit from the $(\bar{N}+0)$ manifold to the $(\bar{N}-1)$ manifold. The first "real" inelastic process is the relaxation to the $|(\widetilde{00-1}),(\widetilde{1-1-2})\rangle$ channel, which opens at $\nu/B = 1$.

Further, here we consider collisional dynamics only in the ultracold regime ($E < E_D$), namely, at temperatures of 1 μK, which usually implies a threshold regime in which dipolar collisions may be described as exhibiting universal behavior [29]. Figure 5 shows the cross sections as a function of the frequency for fermionic prototype molecules; the left panels show cases when molecules are in the lowest (for $\bar{N}+0$ manifold) strong-field-seeking state $|(\widetilde{000})\rangle$ and which is a ground state (see Figs. 1 and 2), while the right panels show cases when molecules are in the first (for this manifold) excited state $|(\widetilde{1-1-1})\rangle$ and which is a weak-field-seeking one at considered field strengths. Two types of pronounced resonance structures are apparent. First, the broad resonances at $\nu/B = 2,4$ reflect the resonance frequencies [and, therefore, the avoided crossings; Fig. 1(a)] between the $|0,0\rangle$ and $|1,-1\rangle$ states, between the $|1,-1\rangle$ and $|2,-2\rangle$ states, and so on. The second type of resonance structure includes a large number of sharp resonances (Feshbach resonances) as a consequence of short-range interactions. These structures will not be considered here because short-range interactions are unknown, and their appearance is defined by the inner wall of the potential. It should be noted that such resonance structure is quite intensive for molecules in the $|(\widetilde{000})\rangle$ state, while it is almost absent for molecules in the $|(\widetilde{1-1-1})\rangle$. The reason for it is quite simple: the dressed adiabatic potential for the $|(\widetilde{1-1-1}),(\widetilde{1-1-1})\rangle$ is always repulsive, which includes a van der Waals repulsion as well, and so is shielded from the short-range region at ultracold temperatures. The inelastic

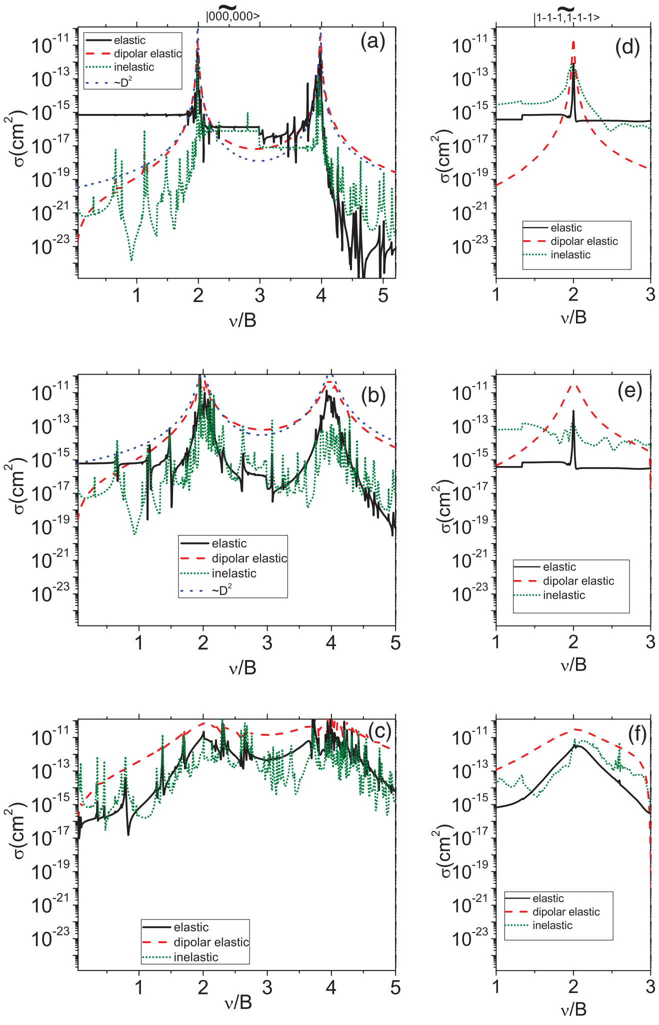

FIG. 5. (Color online) Elastic (solid lines), dipolar elastic (dashed lines), and inelastic (dotted lines) cross sections vs the frequency of the microwave electric field at the collision energy 1 μK for (a), (d) $x = 0.01$, (b), (e) $x = 0.1$, and (c), (f) $x = 0.5$ strengths for the prototype molecules with $\mu = 1$ D. The (a)–(c) cases are for molecules in the $|(\widetilde{000})\rangle$ state; the (d)–(f) cases are for molecules in the $|(1-\widetilde{1}-1)\rangle$ state. See the text for details.

processes are mostly caused by the diabatic crossings, which, as a rule, happen at distances larger than a characteristic scale for short-range interactions $[(\mu^2/B)^{1/3}]$ and limit the barrier height [39,65]. The detailed picture of it will be considered elsewhere.

At small field strengths, such as $x \ll 1$ and out-of-resonance frequencies, the elastic cross sections of the $|(\widetilde{000}),(\widetilde{000})\rangle \Longrightarrow |(\widetilde{000}),(\widetilde{000})\rangle$ [or $|(1-\widetilde{1}-1),(1-\widetilde{1}-1)\rangle \Longrightarrow |(1-\widetilde{1}-1),(1-\widetilde{1}-1)\rangle$] process depend extremely weakly on the frequency [Figs. 5(a) and 5(d)]. The cross sections appear as straight lines, indicating that this type of elastic collision is mainly determined by the short-range components of the interaction potential, and the dipole-dipole interactions are not extensively involved. As we mentioned above, the elastic cross section for molecules in the $|(1-\widetilde{1}-1)\rangle$ state is mostly defined by the repulsive van der Waals interaction in such cases.

The dipolar elastic process almost always dominates the collision dynamics, especially at large field strengths and small detunings around the resonant frequencies. Figure 5 also demonstrates that the dipolar elastic cross sections agree rather well with the universal threshold behavior $\propto D^2$ near the resonance frequency ($\nu = 2B$), where such behavior can be easily determined in the dressed-molecule picture because the effective dipole moment for each molecule is defined as $\sqrt{2}\lambda\Omega\mu/(\lambda^2 + \Omega^2)$ (see, for example, [18]), where $\lambda = (\Delta + \sqrt{\Delta^2 + 4\Omega^2})/2$, $\Delta = \nu - 2B$, and $\Omega = \mu\mathcal{E}/h$ is the Rabi frequency. This agreement is true for any resonance frequency and at not very large field strengths ($x \ll 1$). At large field strengths ($x = 1$, for example), the effective dipole moment and, therefore, the dipole scattering length should not be defined according to this simple formula because the dressed states are a superposition of more than two states.

Ground-state polar molecules can undergo inelastic collisions in the presence of a microwave field, and the collision rates can be quite enhanced. This was demonstrated in [66] using a simple model based on the Born approximation. The same effects were observed in [42] for atom-molecule collisions, and the inelastic rates were found to be enhanced near the avoided crossings between different Zeeman levels. Here, we see the same effects near the resonance frequencies, except for molecule-molecule collisions in which crossings between different Stark levels are avoided. Thus, if the detuning is small (near-resonance frequencies), both elastic and inelastic collisions are enhanced, and the inelastic cross sections can be easily compared with the elastic ones (Fig. 5). Although the near-resonance frequencies provide deep traps, their use may be impractical for evaporative cooling because of the large rate of inelastic collisions. At small field strengths ($x = 0.01$, for example) and at frequencies far from resonance, the inelastic cross sections are indeed small. The reason for this is clear: ground-state molecules are "weakly dressed," and inelastic collisions are "weak" as well. By the same reasoning, however, the dipolar elastic cross sections can be quite small. This does not contribute positively toward effective evaporative cooling, although it can still be helpful.

Another interesting feature arises from the fact that our state of interest is a superposition of $|0,0\rangle$, $|1,-1\rangle$, $|2,-2\rangle$, and similar states. However, at low field strengths, this state is almost a pure $|0,0\rangle$ state at $0 < \nu \ll 2B$ frequencies, almost a pure $|1,-1\rangle$ state at $2B \ll \nu \ll 4B$ frequencies, and so on [Fig. 1(a)]. Moreover, it is possible to achieve rather small inelastic collision rates between these resonance frequencies [Fig. 5(b)]. Thus, to optimize the loading of a microwave trap with molecules, we suggest that it is "safer" to load $|J = 0, M = 0\rangle$ molecules at $\nu/B < 2$; $|1,-1\rangle$ at around $\nu/B = 3$; $|2,-2\rangle$ at around $\nu/B = 5$; and so on, and it would be better to define $x < 1$, which decreases the regions of strong mixing. Although, for example, if the loading of ground-state ($|J = 0, M = 0\rangle$) molecules is at red-detuned frequencies [$\nu/B < 2$; Figs. 5(a)–5(c)], then one can easily catch some of Feshbach resonances, which are especially abundant at near-resonance frequencies $\nu/B = 2,4,\ldots$. On the other hand, if ground-state molecules are loaded at blue-detuned frequencies and the microwave field (MW) is ramped on adiabatically, then the ground state evolves into the state $|(1-\widetilde{1}-1)\rangle$ [$\nu/B > 2$;

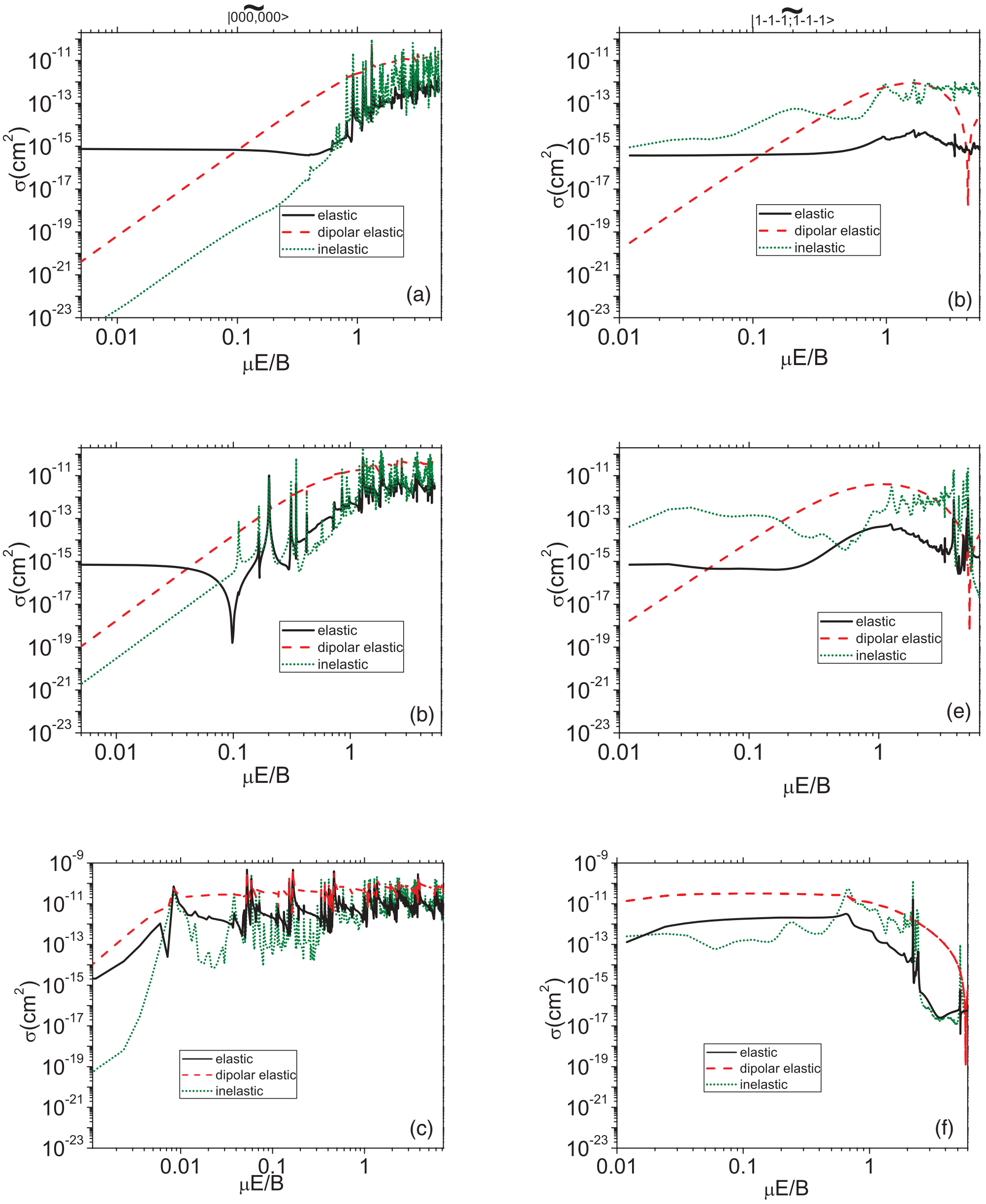

FIG. 6. (Color online) Elastic (solid lines), dipolar elastic (dashed lines), and total inelastic (dotted lines) cross sections vs the microwave electric-field strength at the collision energy 1 μK for (a), (d) $\nu/B = 1$, (b), (e) $\nu/B = 1.5$, and (c), (f) $\nu/B \approx 2$ for the prototype molecules. The (a)–(c) cases are for molecules in the $|(\widetilde{000})\rangle$ state; the (d)–(f) cases are for molecules in the $|(1-\widetilde{1}-1)\rangle$ state.

Fig. 1(a)]; inelastic cross sections can be quite large as well but with less of a resonance structure [Figs. 5(d)–5(f)] because of the shielding described above. At large field strengths ($x > 1$), it may be difficult to obtain a small inelastic cross section [Fig. 5(c)] for molecules with a large dipole moment. To clarify this, we show the dependence of the cross section on the microwave electric-field strength (Fig. 6). One can see that all cross sections are saturated when getting closer to $x = 1$, which reflects the long-range physics of the interacting dipoles. But such behavior is interrupted for molecules in the $|(1-\widetilde{1}-1)\rangle$ state at quite a large value of the MW field, which may denote the existence of some diabatic crossings (Fig. 1). But, regardless, cases with larger fields, $x \gtrsim 1$, have to be verified by taking into account more rotational levels (in our case, we only have $N = 0,1,2$ levels) and will be studied elsewhere. Again, a rich resonance structure is associated with these cross sections and is abundant for molecules initially in the $|(\widetilde{000})\rangle$ state. Saturation occurs at $\mu\mathcal{E} \sim 2hB$ for out-of-resonance frequencies [Figs. 6(a) and 6(c)] and at $\mu\mathcal{E} \sim \Delta$ for near-resonance frequencies [Fig. 6(b)]. In general, inelastic cross sections are comparable to elastic ones at field strengths larger than the saturation field. Thus, it is more practical to choose the field strength considerably smaller than the strength at saturation either for out-of-resonance frequencies or for near-resonance ones. But it should not be very small, such as $x \approx 0.01$, for out-of-resonance frequencies, as the dipole-dipole interaction is not engaged enough and collisional dynamics is mostly defined by short-range interactions.

IV. SUMMARY

In this paper, we describe a theoretical investigation of ultracold collisions among ground-state polar diatomic molecules in a circularly polarized microwave field. Our results show that the collisions are highly sensitive to the external field and can be explained qualitatively and, up to some extent, quantitatively by only knowing the dipole moment and the rotational constant of polar diatomic molecules. The full quantitative description can only be possible if a full short-range potential surface is known. We have found that strong long-range dipole-dipole interactions provide a resonant exchange of internal energy by transitioning between the $|J=0,M=0\rangle$ and $|J=1,M=-1\rangle$ states, between the $|J=1,M=-1\rangle$ and $|J=2,M=-2\rangle$ states, and so on, so that this process determines dipolar elastic collisions. Such dipolar elastic collisions dominate the other collisions at almost any parametrization of the microwave field, and these collisions may facilitate the successful evaporative cooling of polar molecules. However, a rich resonance structure can spoil it for ground-state molecules loaded at red-detuned frequencies. We have found that for molecules loaded at blue-detuned frequencies, shielding may be effective only for near-resonance frequencies and when the field strength is not large compared with a rotational constant. We conclude that it is impractical to use a field strength at which $\mu\mathcal{E} > 2hB$ or $\mu\mathcal{E} < \Delta$ because the inelastic cross section is not small enough to provide a successful evaporative cooling.

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