Cold collisions between boson or fermion molecules

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(Received 11 September 2003; published 21 January 2004)

We theoretically investigate collisions between electrostatically trapped cold polar molecules and compare boson and fermion isotopes. Evaporative cooling seems possible for fermion molecules as the ratio of the collision loss cross section to the elastic collision cross section (R) gets smaller as the molecular temperature T lowers. With boson molecules, R gets larger as T lowers, which makes evaporative cooling difficult. The elastic collision cross section between fermion molecules can be larger than that for boson molecules with certain conditions.

DOI: 10.1103/PhysRevA.69.012709 PACS number(s): 34.50.Ez

I. INTRODUCTION

Since the development of laser-cooling ultracold atoms have been used for time standards and for precision testing of quantum electrodynamics as well as in various other fundamental physics theories. It has also become possible to achieve Bose-Einstein condensation and the atom laser. Not surprisingly, the next step of interest is to get cold molecules. Molecules have much more to offer than simply extending the experiments already performed with atoms to more complex species. The dipole-dipole interaction in a molecular Bose-Einstein condensate shows a new and intriguing property. Polar fermion molecules can be used to observe the superfluid transition.

Since 1998, several different groups have prepared and trapped cold molecules. Through photoassociation of laser cooled atoms, Fioretti *et al.* obtained cold Cs_2 molecules and Nikolov *et al.* achieved K_2 molecules [1,2]. Takekoshi *et al.* trapped Cs_2 molecules produced from the photoassociation of laser-cooled Cs atoms in focused CO_2 laser beams [3]. There is still the problem that molecules constructed by photoassociation always have high vibrational states. However, cold Rb_2 and Cs_2 molecules at ground vibrational states were constructed from Bose-Einstein-condensed atoms using a Feshbach resonance [4,5]. A Harvard group used static magnetic fields to trap paramagnetic CaH molecules precooled by buffer-gas collisions [6,7]. And Bethlem *et al.* decelerated ND_3 molecular beams using a time-varying inhomogeneous electric field, and then loaded them into an electrostatic trap [8].

Evaporative cooling is a useful method for reducing the temperature of trapped molecules. Using only evaporative cooling, Fried *et al.* cooled hydrogen atoms enough to get the Bose-Einstein condensation [9]. To obtain evaporative cooling effect, the elastic collision rate should be high and the trap loss rate low [10]. Only molecules in low-field-seeking states are trapped by a dc electric field, and trap loss is caused by the transition to high-field-seeking states. We analyzed the loss rate of the linear polar molecules in the $^1\Sigma$ ($J=1$, $M_J=0$) state, which are caused by the Majorana effect (the transition between quantum states, caused by a change of the electric-field direction) [11] and the inelastic collision [12,13]. Here, J denotes the quantum number of the total molecular angular momentum and M_J is the quantum number of the trajectory of the molecular angular momentum parallel to the electric field. Evaporative cooling is difficult for boson molecules in the $^1\Sigma(J=1, M_J=0)$ state, because the ratio of the collision loss rate to the elastic collision rate (R) gets higher as the molecular kinetic energy T decreases when $T<100\ \mu$K [13]. Bohn and Avdeenkov showed that evaporative cooling is difficult for cold diatomic polar molecules in the $^1\Pi$ states [14,15].

References [13–15] only discussed boson molecules. The collision between fermions have been considered to be negligible [16–18]. This argument is valid for cold atomic collision. The interatomic short-range force is significant only for the $L=0\rightarrow L'=0$ scattering term, which cannot exist between fermions (L,L': quantum number of the angular momentum of the relative motion before and after the collision, respectively). The situation is quite different for collisions between polar molecules, where the dipole-dipole interaction is dominant. This interaction is not spherically symmetric and the $L=0\rightarrow L'=0$ scattering term is zero. The collision between boson molecules is mostly determined by the $L=0\rightarrow L'=2$, $L=2\rightarrow L'=0$, and $L=2\rightarrow L'=2$ scattering terms, while the $L=1\rightarrow L'=1$ scattering term is the most dominant for fermion molecules. Comparing the possible scattering terms, the collision cross section between fermion molecules seems to be in the same order as that between boson molecules. This paper analyzes the elastic and inelastic collision cross sections of cold polar molecules, and compares boson and fermion isotopes with the same values for the permanent dipole moment μ, rotational constant B, and reduced mass m.

II. CALCULATION OF COLLISION CROSS SECTION

This paper discusses the collision between electrostatically trapped molecules. It is expected that trapped molecules are localized to a single quantum state (Φ_0), where the trapping force is strongest. The cross sections of the collision procedures $|\Phi_0,\Phi_0\rangle\rightarrow|\Phi_1,\Phi_2\rangle$ are obtained from

$$\sigma_{(\Phi_1,\Phi_2)}=\sum_{L,M_L}\sum_{L',M_L'}\eta(L)\sigma[(\Phi_1,\Phi_2)(L,M_L)\rightarrow(L',M_L')],$$

$$\sigma[(\Phi_1,\Phi_2)(L,M_L)\rightarrow(L',M_L')] = \frac{\pi}{k^2}P[(\Phi_1,\Phi_2)(L,M_L)\rightarrow(L',M_L')], \quad (1)$$

where k is the incident wave number. $M_L(M_L')$ are the quantum numbers for the angular momentum trajectory of the relative motion parallel to the electric field before (and after) the collision. P is the opacity function [14].

$\eta(L)$ is a factor to show the effect of the symmetrization of the wave functions. For a collision between different kinds of molecules, $\eta(L)=1$ for all values of L. For a collision between the same kind of molecules, the following transform must be given.

(1) Boson:

$$|\Phi,\Phi'\rangle\rightarrow\frac{1}{\sqrt{2(1+\delta(\Phi,\Phi'))}}(|\Phi,\Phi'\rangle+|\Phi,\Phi'\rangle)$$

$$f(\theta)\rightarrow[f(\theta)+f(\pi-\theta)].$$

(2) Fermion:

$$|\Phi,\Phi'\rangle\rightarrow\frac{1}{\sqrt{2(1+\delta(\Phi,\Phi'))}}(|\Phi,\Phi'\rangle-|\Phi,\Phi'\rangle),$$

$$f(\theta)\rightarrow[f(\theta)-f(\pi-\theta)], \quad (2)$$

where $f(\theta)$ is the scattering amplitude. Values of $\eta(L)$ are given by the following.

(a) Boson:

$$\eta(L)=0 \quad \text{for} \quad L=\text{odd},$$

$$\eta(L)=2 \quad \text{for} \quad L=\text{even}, \quad \Phi_1=\Phi_2,$$

$$\eta(L)=4 \quad \text{for} \quad L=\text{even}, \quad \Phi_1\neq\Phi_2.$$

(b) Fermion:

$$\eta(L)=0 \quad \text{for} \quad L=\text{even},$$

$$\eta(L)=2 \quad \text{for} \quad L=\text{odd}, \quad \Phi_1=\Phi_2,$$

$$\eta(L)=4 \quad \text{for} \quad L=\text{odd}, \quad \Phi_1\neq\Phi_2. \quad (3)$$

If only dipole-dipole interaction is taken into account and the Born approximation is used,

$$\sigma[(\Phi_1,\Phi_2)(L,M_L)\rightarrow(L',M_L')]=\frac{\pi}{k^2}\left|\frac{m\sqrt{kk'}}{\hbar^2}\int H(r,\theta,\varphi)Y^*_{L,M_L}(\theta,\varphi)Y_{L',M_L'}(\theta,\varphi)j^*_L(kr)j_{L'}(k'r)r^2\sin\theta dr d\theta d\varphi\right|^2, \quad (4)$$

where k' denotes the wave number of the scattering wave. The matrix element of the intermolecular Hamiltonian is given by

$$\langle\Phi_0,\Phi_0|H(r,\theta,\varphi)|\Phi_1,\Phi_2\rangle=\frac{1}{4\pi\varepsilon_0 r^3}\langle\Phi_0|\vec{\mu}|\Phi_1\rangle\cdot\langle\Phi_0|\vec{\mu}|\Phi_2\rangle-\frac{3}{4\pi\varepsilon_0 r^5}(\langle\Phi_0|\vec{\mu}|\Phi_1\rangle\cdot\vec{r})(\langle\Phi_0|\vec{\mu}|\Phi_2\rangle\cdot\vec{r}), \quad (5)$$

where $\vec{\mu}$ is the dipole moment vector. Taking the z direction parallel to the electric field, $\vec{\mu}$ is described as

$$\vec{\mu}=\left(\frac{\mu_+ +\mu_-}{2},\frac{\mu_+ -\mu_-}{2i},\mu_z\right)$$

and Eq. (5) is rewritten as

$$\begin{aligned}\langle\Phi_0,\Phi_0|H(r,\theta,\varphi)|\Phi_1,\Phi_2\rangle=&\frac{1}{4\pi\varepsilon_0 r^3}\left(\frac{\langle\Phi_0|\mu_+|\Phi_1\rangle\langle\Phi_0|\mu_-|\Phi_2\rangle+\langle\Phi_0|\mu_-|\Phi_1\rangle\langle\Phi_0|\mu_+|\Phi_2\rangle}{2}+\langle\Phi_0|\mu_z|\Phi_1\rangle\langle\Phi_0|\mu_z|\Phi_2\rangle\right)\\&-\frac{3}{4\pi\varepsilon_0 r^5}\left[\left(\frac{\langle\Phi_0|\mu_+|\Phi_1\rangle e^{-i\varphi}+\langle\Phi_0|\mu_-|\Phi_1\rangle e^{i\varphi}}{2}\right)\sin\theta+\langle\Phi_0|\mu_z|\Phi_1\rangle\cos\theta\right]\\&\times\left[\left(\frac{\langle\Phi_0|\mu_+|\Phi_2\rangle e^{-i\varphi}+\langle\Phi_0|\mu_-|\Phi_2\rangle e^{i\varphi}}{2}\right)\sin\theta+\langle\Phi_0|\mu_z|\Phi_2\rangle\cos\theta\right]. \quad (6)\end{aligned}$$

As $\langle M_J|\mu_\pm|M_J'\rangle$ and $\langle M_J|\mu_z|M_J'\rangle$ are zero except for $\langle M_J|\mu_\pm|M_J\pm1\rangle$ and $\langle M_J|\mu_z|M_J\rangle$, Eq. (6) is described as

$$\langle\Phi_0,\Phi_0|H(r,\theta,\varphi)|\Phi_1,\Phi_2\rangle=\frac{1}{4\pi\varepsilon_0 r^3}S_{\Delta M_{J1},\Delta M_{J2}}(\theta,\varphi),$$

$$|M_{J1},M_{J2}\rangle\rightarrow|M_{J1},M_{J2}\rangle,$$

$$S_{0,0}(\theta,\varphi)=\langle\Phi_0|\mu_z|\Phi_1\rangle\langle\Phi_0|\mu_z|\Phi_2\rangle(1-3\cos^2\theta),$$

$$|M_{J1},M_{J2}\rangle\rightarrow|M_{J1},M_{J2}\pm1\rangle,$$

$$S_{0,\pm1}(\theta,\varphi)=\frac{3}{2}\langle\Phi_0|\mu_z|\Phi_1\rangle\langle\Phi_0|\mu_\pm|\Phi_2\rangle\sin\theta\cos\theta e^{\pm i\varphi},$$

$$|M_{J1},M_{J2}\rangle\rightarrow|M_{J1}\pm1,M_{J2}\pm1\rangle,$$

$$S_{\pm1,\pm1}(\theta,\varphi)=\tfrac{3}{4}\langle\Phi_0|\mu_\pm|\Phi_1\rangle\langle\Phi_0|\mu_\pm|\Phi_2\rangle\sin^2\theta e^{\pm2i\varphi},$$

$$|M_{J1},M_{J2}\rangle\rightarrow|M_{J1}\pm1,M_{J2}\mp1\rangle,$$

$$S_{\pm1,\mp1}(\theta,\varphi)=-\tfrac{1}{4}\langle\Phi_0|\mu_\pm|\Phi_1\rangle\langle\Phi_0|\mu_\mp|\Phi_2\rangle(1-3\cos^2\theta). \tag{7}$$

Equation (4) is calculated as

$$\sigma[(\Phi_1,\Phi_2)(L,M_L)\rightarrow(L',M_L')]=\frac{m^2}{16\pi\varepsilon_0^2\hbar^4}G_{L,L'}\left(\frac{k'}{k}\right)F(\Delta M_{J1},\Delta M_{J2},L,M_L,L',M_L'),$$

$$F(\Delta M_{J1},\Delta M_{J2},L,M_L,L',M_L')=\left|\int S_{\Delta M_{J1},\Delta M_{J2}}(\theta,\varphi)Y^*_{L,M_L}(\theta,\varphi)Y_{L',M_L'}(\theta,\varphi)\sin\theta d\theta d\varphi\right|^2,$$

$$G_{L,L'}\left(\frac{k'}{k}\right)=\frac{k'}{k}\left[\int j_L^*(kr)\frac{1}{r^3}j_{L'}(k'r)\,r^2dr\right]^2=\frac{k'}{k}\left[\int j_L^*(kr)\frac{1}{(kr)}j_{L'}(k'r)d(kr)\right]^2$$

$$\frac{k'}{k}=\sqrt{1+\frac{\Delta E}{T}},$$

$$T=\frac{(\hbar k)^2}{2m},$$

$$\Delta E=2E(\Phi_0)-E(\Phi_1)-E(\Phi_2), \tag{8}$$

where $E(\Phi)$ is the energy of the quantum state Φ and T denotes the molecular kinetic energy. $F(\Delta M_{J1},\Delta M_{J2},L,M_L,L',M_L')$ becomes nonzero only when

$$M_{J1}+M_{J2}+M_L=M_{J1}'+M_{J2}'+M_L',$$

$$L+L'=\text{even number}. \tag{9}$$

Note also that the collision term $L=0\rightarrow L'=0$ does not exist for the dipole-dipole interaction because of $F(\Delta M_{J1},\Delta M_{J2},0,0,0,0)=0$. This paper discusses the collisions taking $L=0,2\rightarrow L'=0,2$ terms for boson and $L=1\rightarrow L'=1,3$ terms for fermion molecules into account.

Equations (1) and (8) show that the elastic collision cross section ($\Phi_1=\Phi_2=\Phi_0$) does not depend on T when the Born approximation is valid. The inelastic collision cross section is a function of k'/k $[=\sqrt{1+(\Delta E/T)}]$. The collisional transition is possible only when $\Delta E+T>0$, so that k' is the real value. The collisional transition is possible only when $\Delta E>0$ for ultralow temperatures. Reference [19] shows a rough relation $G_{L,L'}(k'/k)\propto(k'/k)^{1-2L}$. Figure 1 shows $G_{L,L'}(k'/k)$, which is obtained by numerical calculation. Actually,

$$G_{0,2}\propto(k'/k),$$

$$G_{1,1},G_{1,3}\propto\frac{1}{(k'/k)},$$

$$G_{2,0},G_{2,2}\propto\frac{1}{(k'/k)^3} \tag{10}$$

are valid with $k'/k\gg1$. As the collision loss cross sections are determined mainly by the $L=0\rightarrow L'=2$ term (G_{02}) for boson and $L=1\rightarrow L'=1$ term (G_{11}) for fermion molecules, the dependence of R (ratio of the collision loss rate to the elastic collision rate) on $\Delta E/T$ is given by

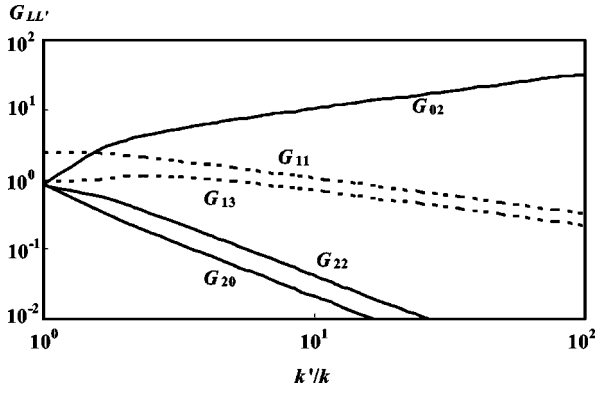

FIG. 1. $G_{LL'}$ determined as Eq. (8) as a function of k'/k. The solid lines show the terms that determine the collision cross section between boson molecules. The dotted lines show the terms that determine the collision cross sections between fermion molecules.

$$R^{boson} \propto \sqrt{\frac{\Delta E}{T}},$$

$$R^{fermion} \propto \sqrt{\frac{T}{\Delta E}}. \tag{11}$$

Equation (11) shows that evaporative cooling is difficult for boson molecules, as R becomes larger as T lowers, as shown in Refs. [13–15]. However, performing evaporative cooling with fermion molecules is rather easy as R gets smaller as T lowers.

Born approximation is used in this paper, which is valid when the following two conditions are satisfied.

(1) The influence of the repulsive force is negligible at $r = 1/k'$, where $1/k'$ is the wavelength of the scattering wave. The molecular wave function should actually be almost zero at $r<d$, where d is the maximum intermolecular distance where the intermolecular repulsive force is significant. As the collisional interaction is caused at $r<\min(1/k,1/k')$, R should be much smaller than the value obtained by the Born approximation when $1/k' = \hbar/\sqrt{2m\Delta E} < d$. Also the distorted-wave Born approximation has been proposed, taking the wave function zero at $r<d$ [20]. Assuming $m=25$ a.u. and $d=0.3$ nm, the influence of the repulsive force is significant when $\Delta E > 140$ mK.

(2) T is low enough so that the $L=0$ (boson) or $L=1$, $M_L=0,\pm 1$ (fermion) scattering terms obtained by the Born approximation are smaller than π/k^2. When T is not low enough for the Born approximation to be invalid, the contribution of the partial waves $L \geqslant 3$ is more significant and R becomes smaller than that obtained by the Born approximation because of $G_{L,L'}(k'/k) \propto (k'/k)^{1-2L}$.

For the collision between boson and fermion molecules, the following relations are valid, as $L+L'$ must be even numbers.

$$\sigma_{elastic}^{bose-fermion} = \frac{\sigma_{elastic}^{boson} + \sigma_{elastic}^{fermion}}{2}, \tag{12}$$

$$\sigma_{loss}^{bose-fermion} = \frac{\sigma_{loss}^{boson} + \sigma_{loss}^{fermion}}{2}, \tag{13}$$

$$R^{boson-fermion} = \frac{\sigma_{loss}^{boson-fermion}}{\sigma_{elastic}^{boson-fermion}} = \frac{\sigma_{loss}^{boson} + \sigma_{loss}^{fermion}}{\sigma_{elastic}^{boson} + \sigma_{elastic}^{fermion}},$$

with $\Delta E \gg T$ and $1/k' > d$

$$\approx \frac{\sigma_{loss}^{boson}}{\sigma_{elastic}^{boson} + \sigma_{elastic}^{fermion}} \propto \sqrt{\frac{\Delta E}{T}}. \tag{14}$$

Equation (14) suggests that the collision loss is significant for the collision between boson and fermion molecules. Evaporative cooling only seems possible for pure fermion molecules.

A. Low-field-seeking molecules

Only molecules in the low-field-seeking states are trapped with a dc electric field. Trap loss is caused by the transition to high-field-seeking states which have a lower energy level ($\Delta E > 0$). More detailed discussions are given for symmetric-top molecules and linear molecules.

1. Symmetric-top molecules without inversion

Here we assume that all molecules are in a vibrational ground state. The initial quantum state of symmetric-top molecules is given by $|\Phi_0\rangle = |J,K_J,M_J\rangle$, where K_J is the quantum number of the rotational angular momentum parallel to the molecular axis. From the dipole selection rule, transitions to $|\Phi\rangle = |J,K_J,M_J \pm 1\rangle$, $|J \pm 1,K_J,M_J\rangle$, $|J \pm 1,K_J,M_J \pm 1\rangle$, and $|J \pm 1,K_J,M_J \mp 1\rangle$ states are possible. However, the $J \rightarrow J+1$ transition is not possible when $T < hB$, as $T+E_0$ is negative. Also the rate of the $J \rightarrow J-1$ transition is expected to be very small because of $1/k' \ll d$, assuming $B>1$ GHz, $m>25$ a.u., and $d \approx 0.3$ nm. We discuss the collision loss just taking $|\Phi\rangle = |J,K_J,M_J \pm 1\rangle$. $|\langle \Phi | \mu_{z,\pm} | \Phi \rangle|^2$ are given by

$$|\langle J,K_J,M_J|\mu_z|J,K_J,M_J\rangle|^2 = \frac{K_J^2 M_J^2}{J^2(J+1)^2}\mu^2, \tag{15}$$

$$|\langle J,K_J,M_J|\mu_\pm|J,K_J,M_J \pm 1\rangle|^2 = \frac{K_J^2(J \mp M_J)(J \pm M_J + 1)}{4J^2(J+1)^2}\mu^2. \tag{16}$$

When molecules in the $|J=1, K_J=1, M_J=1\rangle$ state are trapped by the linear Stark effect, the trap loss is caused by the transition to the $|J=1, K_J=1, M_J=0\rangle$, where there is no linear Stark effect. As two molecules are lost with one collision when $M'_{J1}=M'_{J2}=0$, the collision loss rate σ_{loss} is given by

$$\sigma_{loss} = \sigma_{(M'_{J1}=1,M'_{J2}=0)} + 2\sigma_{(M'_{J1}=0,M'_{J2}=0)}. \tag{17}$$

The collision loss cross section is obtained taking

$$M'_{J1}=1,\ M'_{J2}=0, \quad \Delta E = \tfrac{1}{2}\mu E = U,$$

$$M'_{J1}=0,\ M'_{J2}=0, \quad \Delta E = \mu E = 2U, \tag{18}$$

where E is the electric-field strength and U denotes the trap potential energy.

Assuming $U \gg T$,

$$\sigma_{elastic}^{boson}(\mathrm{cm}^2) = \sigma_{(M'_{J1}=1,M'_{J2}=1)} = 7.75\times 10^{-15}\ \mathrm{m(a.u.)}^2 \mu(\mathrm{D})^4,$$

$$R^{boson} = 13.6 G_{0,2}\left(\sqrt{\frac{U}{T}}\right) + 0.185 G_{0,2}\left(\sqrt{\frac{2U}{T}}\right),$$

$$\sigma_{elastic}^{fermion}(\mathrm{cm}^2) = 2.11\times 10^{-14} m(\mathrm{a.u.})^2 \mu(\mathrm{D})^4,$$

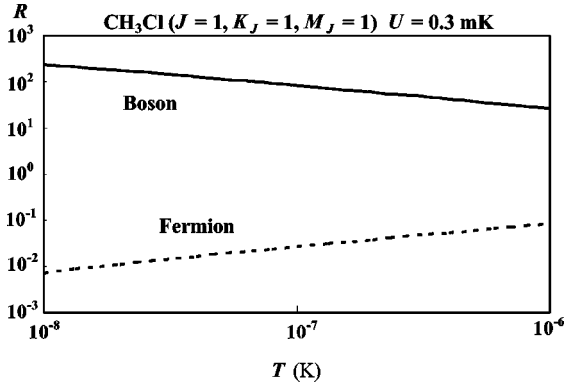

FIG. 2. $R=\sigma_{loss}/\sigma_{elastic}$ for CH_3Cl molecules in the $(J=1, K_J=1, M_J=1)$ state as a function of the molecular kinetic energy T. The trapping potential energy is 0.3 mK, given by an electric field of 15.3 V/cm.

$$R^{fermion}=6.94G_{1,1}\left(\sqrt{\frac{U}{T}}\right)+5.97G_{1,3}\left(\sqrt{\frac{U}{T}}\right)+2.87G_{1,1}\left(\sqrt{\frac{2U}{T}}\right)+4.13G_{1,3}\left(\sqrt{\frac{2U}{T}}\right). \tag{19}$$

For CH_3Cl molecule ($\mu=1.8$ D), the elastic collision cross section is

$$\sigma_{elastic}^{boson}=2.03\times10^{-10}\ \mathrm{cm}^2,$$

$$\sigma_{elastic}^{fermion}=5.53\times10^{-10}\ \mathrm{cm}^2.$$

Figure 2 shows R^{boson} and $R^{fermion}$ as a function of T (<1 μK), taking $U=0.3$ mK ($E=15.3$ V/cm). It shows that $R^{boson}\propto\sqrt{1/T}$ and $R^{fermion}\propto\sqrt{T}$ are actually valid. Fermion isotope is much more advantageous than boson isotope when performing evaporative cooling, because $\sigma_{elastic}^{fermion}>\sigma_{elastic}^{boson}$ and $R^{fermion}\ll R^{boson}$. When $T>1$ μK, the Born approximation is not valid for CH_3Cl molecule and R becomes smaller than the value obtained by Eq. (19).

2. Linear molecules in the $^1\Sigma$ state

In this section we consider linear polar molecules in the $^1\Sigma$ state, which are trapped by the second-order Stark effect. In this case, almost all trapped molecules are in the $|J,M_J\rangle=|1,0\rangle$ state, as $|J,M_J\rangle=|1,0\rangle$ is the lowest low-field-seeking state and the trapping force is strongest. Trap loss is mainly caused by the collisional transition to the $|J,M_J\rangle=|1,\pm1\rangle$, as the $J\rightarrow J+1$ transition is not possible because of $E_0+T<0$ and the $J\rightarrow J-1$ transition is negligibly small because $1/k'\ll d$. We consider taking $|\Phi_0\rangle=|J=1,M_J=0\rangle$ where the trap loss is mainly caused by the transition to the $|\Phi\rangle=|J=1, M_J=\pm1\rangle$ state. Here, $\sigma_{(\Phi_1,\Phi_2)}$ is described as $\sigma_{(M'_{J1},M'_{J2})}$.

For linear polar molecules in the field-free space, the matrix elements of the dipole moment $\langle J,M_J|\mu_z|J,M_J\rangle$ and $\langle J,M_J|\mu_\pm|J,M_J\pm1\rangle$ are zero. However these matrix elements become nonzero under an electric field because of the mixture of wave functions. According to the first-order perturbation theory, the wave function $|J,M_J\rangle$ under an electric field is given by

$$|J,M_J\rangle=|J,M_J\rangle_0+\frac{\langle J,M_J|\mu_z|J-1,M_J\rangle E}{2hBJ}|J-1,M_J\rangle_0-\frac{\langle J,M_J|\mu_z|J+1,M_J\rangle E}{2hB(J+1)}|J+1,M_J\rangle_0, \tag{20}$$

where $|J,M_J\rangle_0$ denotes the wave functions at the field-free space. The matrix elements of the dipole moment are given by

$$|\langle J=1,M_J=0|\mu_z|J=1,M_J=0\rangle|^2=\frac{\mu^4E^2}{25h^2B^2}=\frac{2}{5}\frac{\mu^2}{hB}U,$$

$$|\langle J=1,M_J=0|\mu_\pm|J=1,M_J=\pm1\rangle|^2=\frac{9\mu^4E^2}{400h^2B^2}=\frac{9}{40}\frac{\mu^2}{hB}U,$$

$$U=\frac{\mu^2E^2}{10hB}, \tag{21}$$

where U is the potential energy of the trapped molecule. The energy gap between $|J,M_J\rangle=|1,0\rangle$ and $|1,\pm1\rangle$ is $3U/2$.

Assuming $U\gg T$, Eqs. (1)–(8) are calculated using Eq. (21).

(1) Boson:

$$\sigma_{(0,0)}(\mathrm{cm}^2)=8.7\times10^{-12}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U,$$

$$\sigma_{(0,\pm1)}(\mathrm{cm}^2)=2\times10^{-10}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2\times\left[0.327G_{0,2}\left(\sqrt{\frac{3U}{2T}}\right)+0.327G_{2,0}\left(\sqrt{\frac{3U}{2T}}\right)+0.47G_{2,2}\left(\sqrt{\frac{3U}{2T}}\right)\right],$$

$$\sigma_{(\pm1,\pm1)}(\mathrm{cm}^2)=10^{-10}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2\times\left[0.01G_{0,2}\left(\sqrt{\frac{3U}{T}}\right)+0.01G_{2,0}\left(\sqrt{\frac{3U}{T}}\right)+0.66G_{2,2}\left(\sqrt{\frac{3U}{T}}\right)\right],$$

$$\sigma_{(\pm 1,\mp 1)}(\mathrm{cm}^2) = 2\times 10^{-10}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2 \times\left[0.062G_{0,2}\left(\sqrt{\frac{3U}{T}}\right) + 0.062G_{2,0}\left(\sqrt{\frac{3U}{T}}\right) + 0.094G_{2,2}\left(\sqrt{\frac{3U}{T}}\right)\right].$$

(2) Fermion:

$$\sigma_{(0,0)}(\mathrm{cm}^2) = 2.36\times 10^{-11}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2,$$

$$\sigma_{(0,\pm 1)}(\mathrm{cm}^2) = 2\times 10^{-10}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2 \times\left[0.454G_{1,1}\left(\sqrt{\frac{3U}{2T}}\right) + 0.39G_{1,3}\left(\sqrt{\frac{3U}{2T}}\right)\right],$$

$$\sigma_{(\pm 1,\pm 1)}(\mathrm{cm}^2) = 10^{-10}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2 \times\left[0.44G_{1,1}\left(\sqrt{\frac{3U}{T}}\right) + 0.62G_{1,3}\left(\sqrt{\frac{3U}{T}}\right)\right],$$

$$\sigma_{(\pm 1,\mp 1)}(\mathrm{cm}^2) = 2\times 10^{-10}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2 \times\left[0.074G_{1,1}\left(\sqrt{\frac{3U}{T}}\right) + 0.174G_{1,3}\left(\sqrt{\frac{3U}{T}}\right)\right]. \quad (22)$$

For the boson molecules, the short-range potential ($\propto r^{-6}$) should also be taken into account, particularly when U is not so high. The scattering cross sections caused by the short-range potential are obtained as follows with the assumption that $T\rightarrow 0$ [21]:

$$\sigma^s_{(0,0)}(\mathrm{cm}^2) = \frac{\pi\mu^2}{8\varepsilon_0}\sqrt{\frac{2m}{5h^3B}}\frac{\Gamma^2\left(\frac{3}{4}\right)}{\Gamma^2\left(\frac{5}{4}\right)} = 6.23\times 10^{-13}\mu(\mathrm{D})^2\sqrt{\frac{m(\mathrm{a.u.})}{B(\mathrm{GHz})}},$$

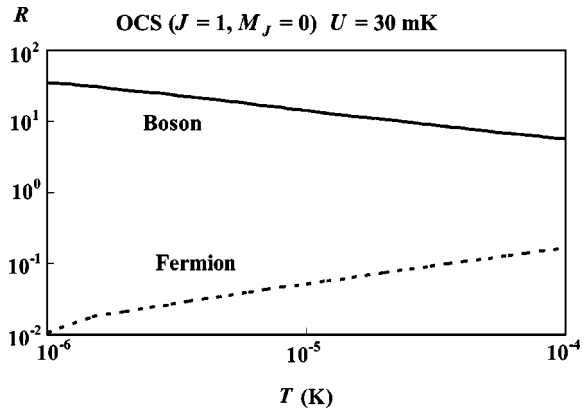

FIG. 3. $R=\sigma_{loss}/\sigma_{elastic}$ for OCS molecules in the ($J=1$, $M_J=0$) state as a function of the molecular kinetic energy T. The trapping potential energy is 30 mK, given by an electric field of 23 kV/cm.

$$\sigma^s_{(\pm 1,\mp 1)}(\mathrm{cm}^2) = \frac{\pi\mu^2}{4\varepsilon_0}\sqrt{\frac{3m}{10h^3B}}\frac{\Gamma^2\left(\frac{3}{4}\right)}{\Gamma^2\left(\frac{5}{4}\right)} = 1.08\times 10^{-12}\mu(\mathrm{D})^2\sqrt{\frac{m(\mathrm{a.u.})}{B(\mathrm{GHz})}}. \quad (23)$$

The elastic collision ($\sigma_{elastic}$) and collision loss (σ_{loss}) cross sections are obtained as follows, by considering that two molecules are lost in one collision with $(M'_{J1},M'_{J2})=(1,1),(-1.-1)$ or $(1,-1)$. Assuming $U\gg T$,

$$\sigma^{boson}_{elastic} = \sigma_{(0,0)} + \sigma^s_{(0,0)},$$

$$\sigma^{boson}_{loss} = \sigma_{(0,1)} + \sigma_{(0,-1)} + 2\sigma_{(1,-1)} + 2\sigma_{(1,1)} + 2\sigma_{(-1,-1)} + 2\sigma^s_{(\pm 1,\mp 1)},$$

$$\sigma^{fermion}_{elastic} = \sigma_{(0,0)},$$

$$\sigma^{fermion}_{loss} = \sigma_{(0,1)} + \sigma_{(0,-1)} + 2\sigma_{(1,-1)} + 2\sigma_{(1,1)} + 2\sigma_{(-1,-1)}. \quad (24)$$

For the OCS molecule ($\mu=0.71$ D, $B=6.09$ GHz) with $U=30$ mK ($E=23$ kV/cm),

$$\sigma^{boson}_{elastic} = 9.6\times 10^{-13}\ \mathrm{cm}^2,$$

$$\sigma^{fermion}_{elastic} = 1.36\times 10^{-13}\ \mathrm{cm}^2.$$

Figure 3 is R^{boson} and $R^{fermion}$ as a function of T (<100 μK). It shows that $R^{boson}\propto\sqrt{1/T}$ and $R^{fermion}\propto\sqrt{T}$ are also valid for linear molecules. For OCS molecule, the Born approximation is valid with higher temperature than CH_3Cl molecules. R^{boson} is smaller than the case of the symmetric-top molecule with the same value of U/T, because also the effect of the short-range force is significant for linear molecules. $R^{fermion}$ is larger than the case of the symmetric -top molecules with the same value of U/T, because

the there are two collisional transitions ($M_J=0\rightarrow M_J'=1$ and $M_J=0\rightarrow M_J'=-1$) which cause the trap loss.

The evaporative cooling of the boson isotope is very difficult also for linear molecules. Also for the fermion isotopes, the evaporative cooling seems more difficult than the symmetric-top molecules as $\sigma_{elastic}^{fermion}$ is small with low U. Taking U larger than a certain value (U_e, shown below), $\sigma_{elastic}^{fermion}$ becomes larger than $\sigma_{elastic}^{boson}$:

$$U_e(\mathrm{K})=0.2\frac{1}{\mu(\mathrm{D})}\left(\frac{B(\mathrm{GHz})}{m(\mathrm{a.u.})}\right)^{3/4}. \tag{25}$$

For the OCS molecule, $U_e=97$ mK (40 kV/cm). With $U=U_e$,

$$\sigma_{elastic}^{boson}=\sigma_{elastic}^{fermion}=1.42\times10^{-12}\ \mathrm{cm}^2.$$

B. $J=0$ state molecules

It recently became possible to trap molecules in high-field-seeking states using a storage ring formed by alternate gradient focusing electrodes [22]. This apparatus is used mainly to trap molecules in the $J=0$ state. The inelastic collisions are impossible when $T\ll hB$. This subsection discusses the elastic collision cross sections taking $|\Phi_0\rangle=|J=0, M_J=0\rangle$. Equations (1)–(8) are calculated using

$$|\langle\Phi_0|\mu_z|\Phi_0\rangle|^2=\frac{\mu^4E^2}{9h^2B^2}=-\frac{2\mu^2}{3hB}U,$$

$$U=-\frac{\mu^2E^2}{6hB}, \tag{26}$$

which is given for all kinds of molecules. For boson isotopes, also the scattering term caused by the short-range potential ($\propto r^{-6}$) given by

$$\sigma_{J=0}^{s}=\frac{\pi\mu^2}{8\varepsilon_0}\sqrt{\frac{2m}{3h^3B}}\frac{\Gamma^2\left(\frac{3}{4}\right)}{\Gamma^2\left(\frac{5}{4}\right)} \tag{27}$$

should be taken into account.

The elastic collision cross sections are given by the following.

(1) Boson:

$$\sigma_{J=0}^{boson}(\mathrm{cm}^2)=8.04\times10^{-13}\mu(\mathrm{D})^2\sqrt{\frac{m(\mathrm{a.u.})}{B(\mathrm{GHz})}}+2.41$$

$$\times10^{-11}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2.$$

(2) Fermion:

$$\sigma_{J=0}^{fermion}(\mathrm{cm}^2)=6.56\times10^{-11}\frac{m(\mathrm{a.u.})^2\mu(\mathrm{D})^4}{B(\mathrm{GHz})^2}U(\mathrm{K})^2. \tag{28}$$

Equation (28) is valid not only for linear polar molecules in the $^1\Sigma$ state but also for all molecules in the $J=0$ state. $\sigma_{J=0}^{fermion}$ is larger than $\sigma_{J=0}^{boson}$ when U is larger than a certain value U_{e0} given by

$$U_{e0}(\mathrm{K})=0.14\frac{1}{\mu(\mathrm{D})}\left(\frac{B(\mathrm{GHz})}{m(\mathrm{a.u.})}\right)^{3/4}. \tag{29}$$

For OCS molecules, $U_{e0}=70$ mK ($E=17$ kV/cm). With $U>U_{e0}$, fermion molecules are more advantageous for performing evaporative cooling. With $U=U_{e0}$,

$$\sigma_{elastic}^{boson}=\sigma_{elastic}^{fermion}=2.06\times10^{-12}\ \mathrm{cm}^2.$$

III. CONCLUSION

Boson atoms are more advantageous than fermion atoms for performing evaporative cooling. This is because atomic collision is caused by a short-range force, which is significant for the $L=0\rightarrow L'=0$ scattering term. As the $L,L'=0$ state does not exist between fermions, the elastic collision rate is much smaller than that for Boson atoms.

Fermions are more advantageous than bosons for performing evaporative cooling for polar molecules in low-field-seeking molecules. The collision between polar molecules is mainly caused by the dipole-dipole interaction, where the $L=0\rightarrow L'=0$ scattering term is zero. As the molecular temperature decreases, the collision loss caused by the $L=0\rightarrow L'=2$ scattering term becomes more significant while the collision losses caused by other scattering terms are reduced. Loss rate caused by the collisions between fermion molecules is much less than that between boson molecules, as the $L=0\rightarrow L'=2$ scattering term does not exist between fermions.

Reference [10] shows that evaporative cooling is effective when $R<1/150$. This condition is satisfied for the Fermion isotope when $U/T>3\times10^4$ (symmetric-top molecules) and 1.2×10^5 (linear molecule) when the Born approximation is valid. We can still get evaporative cooling effect with lower value of U/T when U is so high that the influence of the repulsive force is significant. References [13–15] show that it is difficult to get $R\ll1$ for boson isotopes also taking the influence of the repulsive force into account.

For symmetric-top molecules trapped by the linear Stark effect, the elastic collision rate between fermion molecules is larger than that for boson isotopes. For molecules trapped by the second-order Stark effect (including $J=0$ state molecules), the elastic collision rate between fermion isotopes is larger than boson isotopes with high electric fields.

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