An all-optical velocity filter and beam splitter for generating cold molecular beams: a proposal and simulation

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Abstract

In order to generate one or two cold molecular beams that have neither a permanent electric dipole moment nor a magnetic dipole one, a controllable scheme to form an all-optical velocity filter and molecular beam splitter by using two red-detuned, crossing and cavity-enhanced guiding laser beams is proposed, and both the dynamic velocity filtering and beam splitting processes of the guided cold I\textsubscript{2} molecular beam are studied by using the three-dimensional Monte Carlo method. Our study shows that by adjusting the laser power difference between the two guiding laser beams from \(-124\) W to 124 W, a splitting ratio of the two-arm output molecular beams from about 10.3% to 89.7% can be obtained. Also, by adjusting the intersection angle between the two standing wave cavities from 80° to 10°, an adjustable splitting ratio from about 1.6% to 98.4% can be obtained. If the intersection angle between the guided oblique beam and the guided straight beam is set to 80°, a cold I\textsubscript{2} molecular beam with a full-width at half-maximum longitudinal velocity of 1 m s\textsuperscript{-1} and a longitudinal temperature of 8 mK can be generated by using an all-optical velocity filter.

Keywords: buffer gas cooling, velocity filter, beam splitter

(Some figures may appear in colour only in the online journal)

1. Introduction

In the past 20 years, the field of manipulation and control of cold atoms, macroscopic bodies and molecules has made great progress. Techniques to control and generate ultra-cold or cold atoms [1–3] are very mature due to the implementation of laser cooling, but the preparation of ultra-cold or cold molecules remains difficult due to the complexity of their internal energy level structure. Recently, many issues related to manipulation and control of cold molecules have been addressed experimentally, including electrostatic or optical Stark deceleration [4–10], Zeeman deceleration [11, 12], electrostatic or magnetic velocity filtering [13, 14], electrostatic molecular beam splitting [15], molecular interferometry [16], and so on. It is clear that these methods are only restricted to generating cold molecules with a permanent electric or magnetic dipole moment; that is, the manipulation and control of those molecules (such as I\textsubscript{2} and CH\textsubscript{4}, etc) without a permanent electric or magnetic dipole moment have not been solved well. The manipulation and controlling methods of macroscopic bodies [17–20], in particular, suggest an all-optical velocity filter (AOVF) or an all-optical beam splitter (AOBS) could be used for guided cold molecules, but has not been proposed and demonstrated. However, the generations of cold I\textsubscript{2} and CH\textsubscript{4} molecular beams are very interesting and significant in the field of laser frequency stabilization [21] and frequency standards [22]. So it would be interesting and worthwhile to find an AOVF or AOBS, and use them to generate one or two cold molecular beams without a permanent electric or magnetic dipole moment.

In this paper, an all-optical guiding scheme is proposed to split or filter a cold molecular beam without a permanent
electric or magnetic dipole moment by using two Gaussian laser standing wave fields, which are intersected in standing wave cavities. The dynamical splitting and filtering processes of cold molecules in the AOBS and AOVF are investigated by using a three-dimensional (3D) Monte Carlo method. Here this simulation detail is briefly introduced as follows. In our simulation, a C++ program is used, a Gaussian distribution of pseudo-random number can be produced, and each molecule has six parameters: $x$, $y$, $z$, and $v_x$, $v_y$, $v_z$, which represent its space position and velocity components, respectively. The position and velocity space distributions of incident molecular beam are Gaussian, and the initial position, velocity magnitude and direction of each molecule are random. Molecular movement in the guiding Gaussian laser field will be changed by optical gradient force, with time step $1 \times 10^{-7}$ s, and the position and velocity of the motional molecule at the next step is obtained by Newton’s second law. If the molecule moves out of the light field area it is seen as lost. After moving 20 cm, molecules that are still in the light area are counted as the final signal molecules. The transverse temperature of the output cold molecular beam can be obtained by its transverse velocity distributions, and corresponding longitudinal temperature can be obtained by its longitudinal velocity distribution. We first study the dependences of the velocity distribution of the guided $I_2$ molecular beam and its splitting ratio on the incident laser power, and then analyze the influences of the intersection angle between the two guiding beams on the molecular longitudinal velocity.

2. Scheme and derivations

Our proposed scheme for splitting and filtering buffer gas cooled molecular beams is shown in figure 1. An effusive cold molecular beam with a forward velocity of $45 \text{ m s}^{-1}$ and full-width at half-maximum (FWHM) of $35 \text{ m s}^{-1}$ is formed by buffer gas cooling [23–28]. A single frequency, single mode, high power, red-detuned continuous wave (CW) laser is used to produce two crossing Gaussian laser standing wave fields in the standing wave cavities. The optical system consists of a beam expanding system, beam splitter (BS), mirror $M_1$, $M_2$, $M_3$ and $M_4$, respectively. In order to prevent interference between the two laser beams at a crossing region, we put a $\lambda/2$ wave plate at the front of one standing wave cavity so as to make the polarizations of two laser beams mutually perpendicular. Hence we can regard the light intensity at the intersected point as a superposition of the two laser intensities during our simulations. It is clear from figure 1 that a cold molecular beam output from a buffer gas cooling cell will first be guided by a red-detuned, cavity-enhanced straight Gaussian laser standing wave field, and then be split by both the straight standing wave field and another cavity-enhanced oblique laser one, which form an AOVF for the guided cold molecular beam. In this case, a splitting ratio of such an AOVF can be continuously adjusted by changing the intensity difference of the two guiding laser fields or the intersection angle between the two guiding light fields. On the other hand, due to the straight propagating law of light in free space, one laser beam cannot be used to form an AOVF, but a red-detuned cavity-enhanced oblique laser field can be used to form an AOVF in order to generate a cold molecular beam by changing the direction of the oblique laser field.

Because of the AC Stark effect, cold molecules in the red-detuned laser field undergo a gradient force pointed to the strongest laser intensity, which means that cold molecules are bounded in the transverse direction. Molecular interaction potentials in the red-detuned Gaussian light field are given by $U = -\alpha I/2 \varepsilon_0 c$ [29, 30], where $\alpha$ is the average polarizability of a molecule, $\varepsilon_0$ is the dielectric constant in vacuum, $c$ is the speed of light in vacuum and $I$ is the laser intensity in the optical cavity. In our calculation, the influence of laser detuning on the polarizability of $I_2$ is negligible due to its huge detuning, so $\alpha = 11.6 \times 10^{-40} \text{ C m}^2 \text{ V}^{-1}$ is seen as a constant during our 3D Monte Carlo simulation. Two standing wave cavities are used to enhance the intensity of the guiding laser beam. Cold molecules with proper longitudinal and transverse velocities will be guided along the laser beams after being ejected from the buffer gas cell. Those molecules guided along the straight laser beam are velocity filtered in the transverse direction; some molecules guided along the oblique one are also velocity filtered in both the transversal and longitudinal directions. In our scheme, the laser power can be adjusted from 0 W to 125 W, and the intersection angle is also continuously adjustable from $10^\circ$ to $80^\circ$.

Before Monte Carlo simulation, the cavity enhancement factor was calculated based on standing wave cavity theory [31]. As we know, two counterpropagating laser beams with
the same polarization, frequency and amplitude could form a standing wave field. As shown in figure 1, in the standing wave cavity, if the cavity length is equal to an exact multiple of half the wavelength, it will be resonant with the cavity and then form a standing wave in the cavity. The amplitude reflectivity of mirrors are $r_1$ and $r_2$, respectively. $E$ is the amplitude of the incident laser field and $I$ is its laser intensity, which can be expressed as

$$I(\vec{r}) = \frac{1}{2} |E(\vec{r})|^2.$$  \hspace{1cm} (1)

The first incident laser beam transmitted in the forward direction $z$ has amplitude $E_0$. After each reflection by mirror $M_1$, the amplitude is expressed as

$$E_i = E_0 r_1 r_2 \exp(ik \times 2L),$$

$$E_i = E_n r_1 r_2 \exp(ik \times 2L),$$

and the total amplitude of the forward propagation laser in the plane-concave cavity is given by

$$E_+ = E_0 \sum_{n=0}^{\infty} [r_1 r_2 \exp(ik \times 2L)]^n,$$  \hspace{1cm} (3)

so the total forward propagating laser intensity is

$$I_+ = E_+ E_+^* = \frac{I_0}{1 - r_1 r_2 \exp(ik \times 2L)},$$  \hspace{1cm} (4)

and if $\cos(k \times 2L) = 1$, we obtain a resonance cavity and

$$I_+ = \frac{I_0}{1 + (r_1 r_2)^2 - 2r_1 r_2}.$$  \hspace{1cm} (5)

The counterpropagating light field has equal amplitude to the forward one but opposite phase. Their overall standing wave field is superimposed to be

$$E_{\text{tot}} = [E_+ \exp(ikx) + E_- \exp(-ikx)] \exp(-iwr).$$  \hspace{1cm} (6)

The total intensity of the standing wave field is

$$I = E_{\text{tot}} E_{\text{tot}}^* = 2I_+ [1 - \cos(2kx)],$$  \hspace{1cm} (7)

and the averaged laser intensity in the cavity is given by

$$T = \int_{0}^{2\pi} 2I_+ [1 - \cos(2kx)] d(kx) = \frac{2I_0}{1 + (r_1 r_2)^2 - 2r_1 r_2},$$  \hspace{1cm} (8)

and so the cavity enhancing factor can be written as

$$E_{\text{cav}} = \frac{T}{I} = \frac{2(1 - r_1^2)}{1 + (r_1 r_2)^2 - 2r_1 r_2}.$$  \hspace{1cm} (9)

If $r_1 = 99.95\%$, and when the amplitude reflectivity of the mirror is $r_2 = 99.95\%$, the maximum cavity enhancement factor $E_{\text{cav}} = 2000$ can be obtained, according to equation (9). Taking into account the case of a real experiment, we take $E_{\text{cav}} = 1600$ [32] in our simulation.

3. Results

3.1. An all-optical molecular beam splitter for producing two cold molecular beams

It is clear from figure 1 that a straight guiding laser beam and an oblique guiding laser beam are used to form an AOBS for optically guided molecular beams. In other words, if the output cold molecular numbers from the two guiding laser beams are counted at the same time, our proposed scheme can be regarded as an AOBS. Here we first study the dependences of the splitting ratio of our proposed AOBS on both the intersection angle and the power difference between the incident laser beams of the two standing wave cavities, and the simulated results are shown in figure 2. In figure 2(a), the angle between the two cavities was set to $10^\circ$ and the laser...
power difference $\Delta P = P_{\text{straight}} - P_{\text{oblique}}$ was set as a horizontal coordinate, where $P_{\text{straight}}$ is the incident laser power of the straight laser beam and $P_{\text{oblique}}$ is the incident laser power of the oblique laser beam. We can see from figure 2(a) that by adjusting the incident laser power difference from $-124 \text{ W}$ to $124 \text{ W}$, and when the intersection angle between the two standing wave cavities is $10^\circ$, a controllable AOBS with a continuously adjustable splitting ratio from 10.3% to 89.7% can be formed by using the two red-detuned, crossing and cavity-enhanced laser beams. It is clear from figure 2(b) that when the incident laser power of the straight laser beam is $5 \text{ W}$ and the oblique incident laser power is $120 \text{ W}$, the splitting ratio can be adjusted from 1.6% to 98.4% with an increase of the intersection angle from $10^\circ$ to $80^\circ$. This shows that our proposed all-optical scheme can be used to realize efficient splitting of a cold molecular beam.

3.2. An all-optical velocity filter for generating a cold molecular beam

We can also see from figure 1 that when an oblique guiding laser beam is only used, and its power and oblique direction are changed respectively, an AOVF will be formed. In other words, if the output cold molecular numbers from the oblique guiding laser beam is only counted, our proposed scheme can be regarded as an AOVF. Here we simulate the dynamic filtering process of our proposed AOVF investigated by using a 3D Monte Carlo method, and study the transverse spatial and velocity distributions of the oblique molecular beam for different incident laser power and the dependences of its transverse temperature on the laser power of the oblique incident laser beam. The corresponding results are shown in figure 3. We find from figure 3(a) that with increasing guiding length, the number of guided molecules varies with changing guiding length. The inset illustration on the upper right shows the amplified dependence of the guided molecular number on the guiding length from 150 mm to 200 mm, and the solid curves are obtained by exponential decay fitting. (b) Transverse spatial distribution of the filtered I$_2$ beam in the oblique laser beam for different incident laser power where the intersection angle is $30^\circ$. The inset illustration on the upper right shows the amplified velocity distributions with an incident laser power of 1 W and 5 W, and the curve is obtained by Gaussian fitting. (c) Transverse velocity distribution of the filtered I$_2$ beam in the oblique laser beam for different incident laser power where the intersection angle is $30^\circ$. The inset illustration on the upper right shows the amplified velocity distributions with incident laser power of 1 W, 5 W and 20 W, and the curve is obtained by Gaussian fitting. (d) Dependence of the transverse temperature of the guided cold I$_2$ beam on the incident laser power; the line is obtained by linear fitting.
laser power from 1 W to 100 W, which is because the transverse trapping potential of the oblique laser beam for I$_2$ molecules increases with increasing incident laser power. Figure 3(d) shows a linear dependence of transverse temperature of the guided cold molecular beam on incident laser power, which can be explained by the linear relationship between the optical potential depth and the incident laser power. In particular, when the incident laser power is 1 W, the lowest transverse temperature is about 1 mK. Our further study finds that the incident laser power of the oblique laser beam can only be used to change its transverse temperature, but cannot be used to change its longitudinal temperature.

In addition, the relationship between the longitudinal velocity distribution of the oblique molecular beam for different intersection angles and the dependence of its longitudinal temperature on the intersection angle were also studied when the incident laser power is 100 W, and the simulated results are shown in figure 4. It can be seen from figure 4(a) that by adjusting the intersection angle between the two standing wave cavities (i.e. by changing the direction of the oblique laser beam) from 10$^\circ$ to 60$^\circ$, the central velocity of the generated cold molecular beam (i.e. the oblique molecular beam) and its longitudinal velocity distribution are moved towards the low speed region. Also, figure 4(b) shows the linear dependence of the longitudinal temperature of the resulting cold molecular beam on cos$^2$θ. This can be explained by the formula $k_B T = m \times (v \cos \theta)^2$ which $k_B$ is the Boltzmann constant, $m$ is the relative atomic masses of I$_2$, $v$ is the velocity of molecule and $v \cos \theta$ is the velocity’s projection in the oblique beam. Molecules with $v \cos \theta = v$ are most probably guided by the oblique laser beam. It is clear from figure 4 that when the intersection angle between the two guiding laser beams is 60$^\circ$, we can generate a cold I$_2$ molecule beam with FWHM of about 7 m s$^{-1}$ and a longitudinal temperature of about 380 mK. Further increasing the intersection angle to 80$^\circ$, the FWHM of the molecule beam output from the oblique one can be as low as 1 m s$^{-1}$ and a longitudinal temperature of about 8 mK can be reached. Such a cold I$_2$ molecular beam is very useful in research of frequency standards [22]. This shows that our proposed AOVF can be used to generate a cold molecular beam with a transverse temperature of about 1 mK and a longitudinal temperature of about 8 mK.

In our scheme, the buffer gas cooling technique can be used to generate cold I$_2$ molecular beams [23–28]. This method to produce cold molecular beams is very mature and suitable for almost all chemically stable molecules. The reflecting mirrors and single frequency, single mode, high power laser are also commercially available [32, 33]. To conveniently adjust the intersection angle between two standing wave cavities, we arrange reflecting mirror M$_1$ and M$_3$ outside the vacuum chamber. Here we can use the laser-induced fluorescence technique to probe the molecular signals. So our proposed AOVF and AOBS schemes are feasible in experiment and can be used to generate one or two cold molecular beams.

4. Conclusion

We have proposed simple, controllable and efficient AOVF and AOBS techniques for generating one or two cold molecular beams by using a single frequency, single mode, high power CW laser and two standing wave cavities, and studied the velocity filtering and beam splitting dynamic processes of the resulting cold molecular beams by using a 3D Monte Carlo method. Our investigation shows that the proposed AOBS can be used to conveniently adjust its splitting ratio from 10.3% (1.6%) to 89.7% (98.4%) by changing the incident laser power difference of the two guiding laser beams or by adjusting the intersection angle of the molecular beam splitter. Also, our proposed AOVF can be used to generate a cold molecular beam with a transverse temperature of ∼1 mK and a longitudinal temperature of ∼8 mK. In particular, our proposed all-optical filter and splitter schemes can be used to produce one or two cold molecular beams without a permanent electric dipole moment or a magnetic dipole one (such as I$_2$ and CH$_4$) for further applications in the fields of laser frequency stabilization [21] and frequency standards [22].

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References


[33] Engin D, Lu W, Akbulut M, McIntosh B, Verdun H R and Gupta S 2011 1 kW cw Yb-fiber-amplifier with <0.5 GHz linewidth and near-diffraction limited beam-quality, for coherent combination application Proc. SPIE 7914 791407