Time-dependent approach to the double-channel dissociation of the NaCs molecule induced by pulsed lasers*

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The dynamics of the double-channel dissociation of the NaCs molecule is investigated by using the time-dependent wave packet (TDWP) method with the "split operator-Fourier transform" scheme. At a given wavelength and intensity of laser pulse, the population of each state changing with time is obtained. The photo-absorption spectra and kinetic-energy distribution of the dissociation fragments, which exhibit vibration-level structure and dispersion of the wave packet, respectively, are also obtained. The results show that by increasing the laser intensity, one can find not only the band center shift of the photo-absorption spectrum, but also the change of the fragment energy. The appearance of the diffusive band in the photo-absorption spectrum and the multiple peaks in the kinetic-energy spectrum can be attributed to the effects of the predissociation limit and the external field.

Keywords: time-dependent wave packet method, photo-dissociation dynamics, photo-absorption spectrum, kinetic-energy spectrum, NaCs

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1. Introduction

In the investigation of light-molecule interaction, the dissociation of molecules has always been a very important topic, due to its significance in understanding both the nature of the potential energy curve (PEC) and the mechanism of the bond breaking process.[1] What is more, the progress of the photo-dissociation technique has made many new phenomena, such as multi-channel dissociation,[2] coherent control of dissociation,[3,4] photoassociation reaction,[5–7] etc observed and investigated. Among them, an interesting phenomenon is the double-channel dissociation.

For double-channel dissociation, because it can provide us with the information about spin–orbit coupling, an accurate description of which is essential for a quantitative comparison with experiments, more attention has been paid to it in recent decades.[8–10] In the study of the NaI molecule, Alekseyev *et al.*[10] showed that the inclusion of the spin–orbit coupling can nearly quantitatively reproduce the observed peaks in the absorption spectrum. In the relevant theoretical treatment, the avoided crossing is a common topic for discussion, the existence of which can give rise to some interesting features in time-resolved dynamics. In the process of double-channel dissociation, the existence of the predissociation limit and the overlap region between discrete energy levels of the lower excited state and continuous energy levels of the higher excited state can result in the diffusion of absorption spectrum bands.[11] These phenomena, often occurring in heteronuclear alkali dimers, have been investigated experimentally or theoretically.[12,13]

The alkali-metal atoms, because of their important role in ultracold physics and chemistry, have been frequently investigated in recent years. When these atoms form cold molecules and are induced into their lower vibrational states by external fields, they have opportunities to be ionized or dissociated. Some researchers have done excellent work on these laser-induced processes.[14–16] As a typical cold molecule, NaCs has gradually become the topic of some experimental and theoretical researches in recent years, since it has the largest measured dipole moment in all of the diatomic alkali molecules. In 1986, Sharma *et al.*[17] conducted an experiment on the photo-dissociation of NaCs for the first time. The ratio of dissociation rates was obtained in the study of the predissociation and collisional depopulation of the NaCs excited state by Shen and Li[18] in 2002. They showed that the branching is strongly detuning-dependent in the vicinity of the NaCs near-wing satellite. In 2007, Aymar and Dulieu[19] reported first their calculated transition dipole moments, which laid a foundation for the study of the dissociation dynamics for the NaCs molecule. In the investigation of the two-step photoassociation of some cold molecules,[7,20–22] it was found that the photo-dissociation is also a crucial process. The intensive theoretical and experimental researches on alkali-metal-atom molecules[7,23] showed that because of the features of their PECs, they have great possibilities to be dissociated through the double channels when being in the electronic ground state and exposed to laser fields. So in the study of the external field effect on photo-dissociation dynamics, one often chooses the

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alkali-metal-atom molecules as a study object.

In the theoretical research on the photo-dissociation process, the often-used methods include the classic trajectory method, the quasi-classical trajectory method, the time-dependent wave packet (TDWP) method, and the time-independent method. Among them the TDWP method has been proved to be an effective approach to solving the light-molecule interaction.[24–26] Its advantages over other methods are shown not only in the high efficiency of the numerical calculation, but also in the intuitive picture of the dynamics. In addition, the TDWP method is especially suitable for the study of the real-time dynamics. It has given excellent results in the investigation of photo-ionization,[27] photo-dissociation,[28–30] photoassociation,[7] etc.

In the present work, we choose the NaCs molecule as a study object, and use the TDWP method to explore its photo-dissociation dynamics. The rest of this paper is arranged as follows. In Section 2, the theoretical model of the quantum wave packet method for photo-dissociation, together with the method used to calculate the population in each electronic state, the photo-dissociation absorption spectrum, and kinetic-energy spectrum, is described. In Section 3, we present the results and discuss the effect of an external laser field on the nature of photo-dissociation. The influences of the existence of the predissociation limit and the avoided crossing on the properties of photo-dissociation are also involved in this part. Our concluding remarks are given in Section 4.

2. Method

Consider a three-state system. The radial time-dependent Schrödinger equation of the system within the Born–Oppenheimer approximation, with the coupling of rotations with other degrees of freedom neglected, has the form of

$$\mathrm{i}\hbar\frac{\partial\Psi(R,t)}{\partial t}=(T+V)\Psi(R,t), \tag{1}$$

where $\Psi(R,t)$, T, and V are, respectively, the time-dependent nuclear wave function, the kinetic matrix, and the potential matrix. They can be explicitly expressed as

$$\Psi(R,t)=\begin{pmatrix}\Psi_{\mathrm{X}}(R,t)\\ \Psi_{\mathrm{A}}(R,t)\\ \Psi_{\mathrm{B}}(R,t)\end{pmatrix}, \tag{2}$$

$$T=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial R^2}\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},$$

$$V=\begin{pmatrix}V_{\mathrm{X}}&W_{\mathrm{XA}}&W_{\mathrm{XB}}\\W_{\mathrm{XA}}&V_{\mathrm{A}}&V_{\mathrm{AB}}\\W_{\mathrm{XB}}&V_{\mathrm{AB}}&V_{\mathrm{B}}\end{pmatrix}, \tag{3}$$

where R is the internuclear separation; $\psi_{\mathrm{X}}(R,t)$, $\psi_{\mathrm{A}}(R,t)$, and $\psi_{\mathrm{B}}(R,t)$ are the time-dependent nuclear wave functions in the ground (X) and excited (A, B) states, respectively; m is the reduced mass; V_i $(i=\mathrm{X},\mathrm{A},\mathrm{B})$ refer to the potential functions for the three neutral electronic states $\mathrm{X}^1\Sigma^+$, $\mathrm{A}^1\Sigma^+$, and $\mathrm{B}^1\Sigma^+$ respectively;[19] $W_{ij}=\mu_{ij}E(t)$ $(i,j=\mathrm{X},\mathrm{A},\mathrm{B})$ denote the coupling between the involved electronic states with dipole matrix elements μ_{ij} and external field $E(t)$; V_{AB} is the non-adiabatic coupling.

Given the wave packet $\Psi(R,t_0)$ at initial time t_0, with the split-operator-Fourier scheme of wave packet propagation, the canonical solution of Eq. (1) can be written up to second-order approximation as[31]

$$\Psi(R,t_0+\Delta t)\approx U_V^{1/2}U_TU_V^{1/2}\Psi(R,t_0), \tag{4}$$

where Δt is a small time interval, and

$$U_V=\exp\left[-\frac{\mathrm{i}\Delta t}{\hbar}V(R,t_0)\right],\quad U_T=\exp\left[-\frac{\mathrm{i}\Delta t}{\hbar}T\right], \tag{5}$$

are called the potential- and kinetic-energy evolution operators, respectively. After propagating n steps, the wave function assumes to have the form of

$$\Psi(R,t_0+n\Delta t)\approx\left[\prod_{k=0}^{n-1}U_TU_V(R,t_0+k\Delta t)\right]\Psi(R,t_0). \tag{6}$$

The population of each state can be extracted from the norm of the nuclear wave packet $\Psi_i(R,t)$ $(i=\mathrm{X},\mathrm{A},\mathrm{B})$, i.e.[25]

$$P_i(t)=\int_{R_1}^{R_2}\mathrm{d}R\,|\Psi_i(R,t)|^2, \tag{7}$$

where R_1 and R_2 define the range of inter-nuclear distances. With the wave packet $\Psi_i(R,t)$ $(i=\mathrm{X},\mathrm{A},\mathrm{B})$, other associated information can also be obtained.

In the calculation of TDWP for scattering systems, an often encountered problem is the artificial boundary reflection from the end of the numerical grid, which can distort and ruin the correct dynamics.[32] To eliminate this boundary reflection, in this work, we define an absorbing potential (or optical potential) by[33]

$$V_{\mathrm{abs}}=\begin{cases}-\mathrm{i}V_{i0}\left(\dfrac{R-R_{\mathrm{abs}}}{\Delta R_{\mathrm{abs}}}\right)^n, & R_{\mathrm{abs}}\le R\le R_{\mathrm{abs}}+\Delta R_{\mathrm{abs}},\\ 0, & R<R_{\mathrm{abs}},\end{cases} \tag{8}$$

where V_{i0} is the height of the absorbing potential; R_{abs} is the point far away from the interaction region, at which the absorption is switched on, and ΔR_{abs} is the width of the absorbing potential.

When the wave packet is obtained, the dissociation probability in each channel can be calculated from the probability flux of the wave function at the nuclear separation R_{abs},

$$J_i(t)=\frac{\hbar}{m}\mathrm{Im}\left[\Psi_i^*(R,t)\frac{\partial\Psi_i(R,t)}{\partial R}\right]_{R=R_{\mathrm{abs}}}. \tag{9}$$

If we write the outgoing wave-packet in terms of a real amplitude A and a real phase Φ, i.e.

$$\Psi_i(R,t)=A_i(R,t)\exp[\mathrm{i}\Phi_i(R,t)], \tag{10}$$

then the current density can be written as[33]

$$J_i(R,t) = \frac{|A_i(R,t)|^2}{m} \nabla \Phi_i(R,t). \tag{11}$$

The dissociation yield of fragments, D, is given by the following integration along the nuclear flux direction at $R_{\rm abs}$

$$D(t) = \int_0^t {\rm d}t' J_i\left(R_{\rm abs}, t'\right). \tag{12}$$

Using the expression of momentum distribution[34]

$$\left.\frac{{\rm d}N}{{\rm d}p}\right|_{p'} = \frac{J_i(R_{\rm abs}, t(p'))}{\left|\frac{{\rm d}p}{{\rm d}t}[t(p')]\right|}, \tag{13}$$

where p' is the momentum at which the derivative is calculated, the kinetic-energy distribution has the form of

$$\left.\frac{{\rm d}N}{{\rm d}E}\right|_{p'} = \sqrt{\frac{2m}{T'}} \left.\frac{{\rm d}N}{{\rm d}p}\right|_{p'=\sqrt{2mT'}}. \tag{14}$$

Then in channel i, the photo-absorption spectrum as a function of the photo energy $\hbar\omega$ can be determined by the partial cross section[10]

$$\sigma_i(\omega) = \frac{4\pi^3}{3c\varepsilon_0 m} k_i \omega |\Psi_i(E)|^2, \tag{15}$$

where the wave packet $\Psi_i(E)$ at $R_{\rm abs}$ is Fourier transformed from time domain as

$$\Psi_i(E) = \frac{1}{2\pi} \int_0^\infty \Psi_i(R_{\rm abs}, t) \exp(-{\rm i}Et/\hbar)\, {\rm d}t, \tag{16}$$

$k_i = \sqrt{2m(E - V_i(R_{\rm f}))}/\hbar$ is the wave vector in channel i, $V_i(R_{\rm f})$ is the potential energy in channel i at $R = R_{\rm f}$, and ε_0 is the permittivity of free space.

3. Results and discussion

The present photo-dissociation of NaCs[19] involves three electronic states, i.e. the ground state $X^1\Sigma^+$, and two excited states $A^1\Sigma^+$, $B^1\Sigma^+$ (Fig. 1). As shown in Fig. 1, for excited states $A^1\Sigma^+$ and $B^1\Sigma^+$, besides the existence of an avoided crossing at the inter-nuclear distance about 10.3 au (the unit au is the abbreviation for atomic unit), there is also an overlap region between discrete energy levels of the lower excited state $A^1\Sigma^+$ and continuous energy levels of the higher excited state $B^1\Sigma^+$. These features of the PECs make the dissociation of the NaCs molecule more interesting, especially when one of the excited states is repulsive.

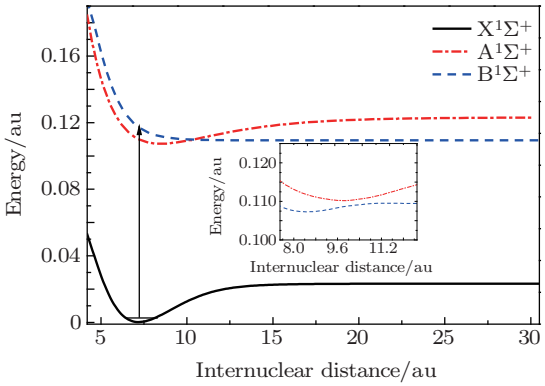


Fig. 1. (color online) Diabatic and adiabatic (lines in the inset, only containing the excited states) PECs for NaCs.

When NaCs molecules in an electron ground state are pumped into excited states by an appropriate laser pulse, the near resonance may happen to states $A^1\Sigma^+$ and $B^1\Sigma^+$, and the molecules may dissociate through two channels, i.e. the upper channel (the dash–dotted line) and the lower one (the dashed line). The calculated dissociation probability changing with time is shown in Fig. 2. Obviously for the lower dissociation channel, there is some plateau regions appearing in the probability curve, which can be explained by the evolution of the wave packet on the potential curve: the wave packet is pumped into the region between the two excited PECs and causes the near resonance with the states $A^1\Sigma^+$ and $B^1\Sigma^+$. For the upper adiabatic state, when the wave packet reaches the position of the avoided crossing from the left turning point, part of it transmits across this region and dissociates through the lower channel. At the same time another part of it moves forward along the potential well until reaching the right-hand-side turning point and then goes back. When the returning wave packet reaches again the crossing position, part of it will transmit across this region and take part in the dynamics on the lower adiabatic path, meanwhile another part of it will go on propagating along the upper adiabatic path until reaching the left turning point. Now it completes the first period of the oscillation. For the lower adiabatic state, the wave packet has a similar behavior except the predissociation through the lower channel. With the movement of the wave packets along their respective potential curves, these dynamic processes recur periodically, and form the plateau regions in the probability curve. However due to the specialty of the PECs, the constrain of the resonance condition and the small Frank Condon factors make the dissociation probability via the upper channel (the dash–dotted line in Fig. 2, shown in the inset is the amplified one) become almost zero.

In order to understand the effect of the laser wavelength on the population transfer between the states, we give the populations of each state, each as a function of time, for different laser wavelengths at laser-intensity $I = 8 \times 10^{14}$ W/cm^2 in Fig. 3. One can see from the figure that the population of each state changes with the laser wavelength increasing from 390 nm to 420 nm. This changing tendency is the direct result

of the near resonance occurring due to the external field and correlated states. Another common feature of the figure is that due to the superposition of the involved energy eigenstates, there is a strong Rabi oscillation in the population with the time evolution from 25 fs to 100 fs. These patterns are consistent with the investigations of the Rabi oscillation of NO in the laser field by Meng *et al.*[35] After the laser field is removed, the Rabi oscillation will disappear; however in the two excited states other kinds of oscillations still exist because of the existence of the coupling of the two excited states. Undoubtedly the study of the Rabi oscillation is helpful to apprehend the nature of the dynamic process.

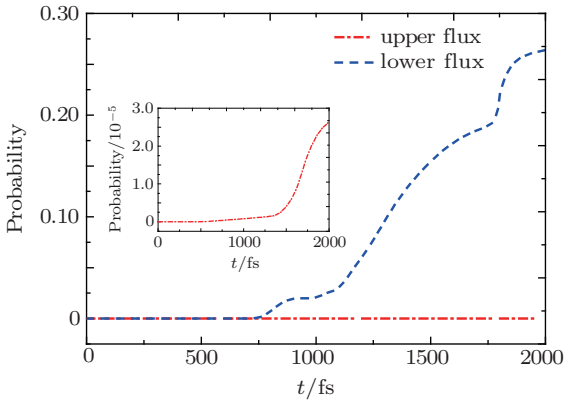


Fig. 2. (color online) Dissociation probabilities of the two channels, the upper channel (the dash–dotted line) and the lower channel (the dashed line), each as a function of time.

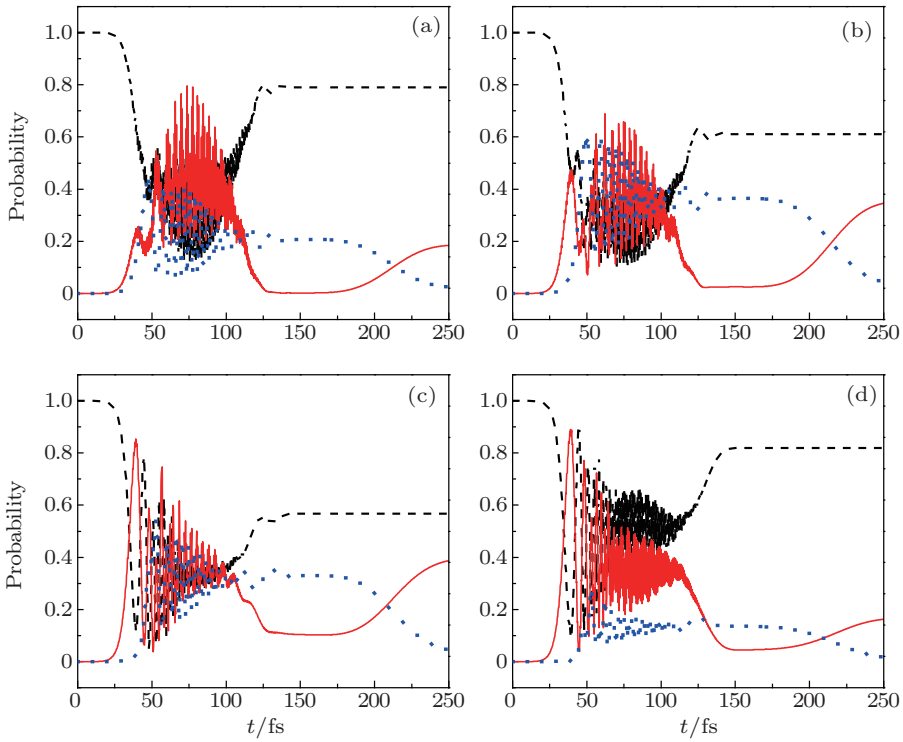


Fig. 3. (color online) The populations of each state (the dashed, solid, and dotted lines denote the ground state $X^1\Sigma^+$ and the excited states $A^1\Sigma^+$, $B^1\Sigma^+$) at different laser wavelengths and intensities of $I = 8 \times 10^{14}$ W/cm^2, each as a function of time: ((a) $\lambda = 390$ nm, (b) $\lambda = 400$ nm, (c) $\lambda = 410$ nm, (d) $\lambda = 420$ nm).

Figure 4 shows the kinetic energy distributions of the dissociative fragments in the lower channel for laser intensities ranging from 8×10^{11} W/cm^2 to 8×10^{14} W/cm^2. At an intensity of 8×10^{11} W/cm^2 (Fig. 4(a)), the dissociation fragments with the largest distribution have a kinetic energy of 0.020 eV. With the laser intensity increasing to 8×10^{12} W/cm^2, the corresponding kinetic energy of the fragments would be 0.016 eV, but the dissociation probability increases drastically (Fig. 4(b)). An increase of the laser intensity will then lead to the similar changes of the fragment energy and the dissociation probability. This scenario is consistent with the investigations of H_2^+ fragmentation reported by Feuerstein and Thumm.[33] The change of the fragment energy with the laser intensity can be elucidated by the external field modified PECs, in other words, the external field modified PECs can lead to the change of the dissociation energy. The origin of the peaks appearing in the kinetic-energy distribution of dissociation fragments can be explained by the dispersion of the wave packet when it evolves in the dissociative channel as described in Ref. [23]. Since the wave packet is not an eigenstate of the coupled Hamiltonian in Eq. (1), it disperses amplitude in the covalent state during the propagation, in other words the modified PEC can distort the wave packet evolving on the upper adiabatic potential well. For the upper channel, however, because of the existence of the predissociation limit, there is almost no fragment produced in this channel.

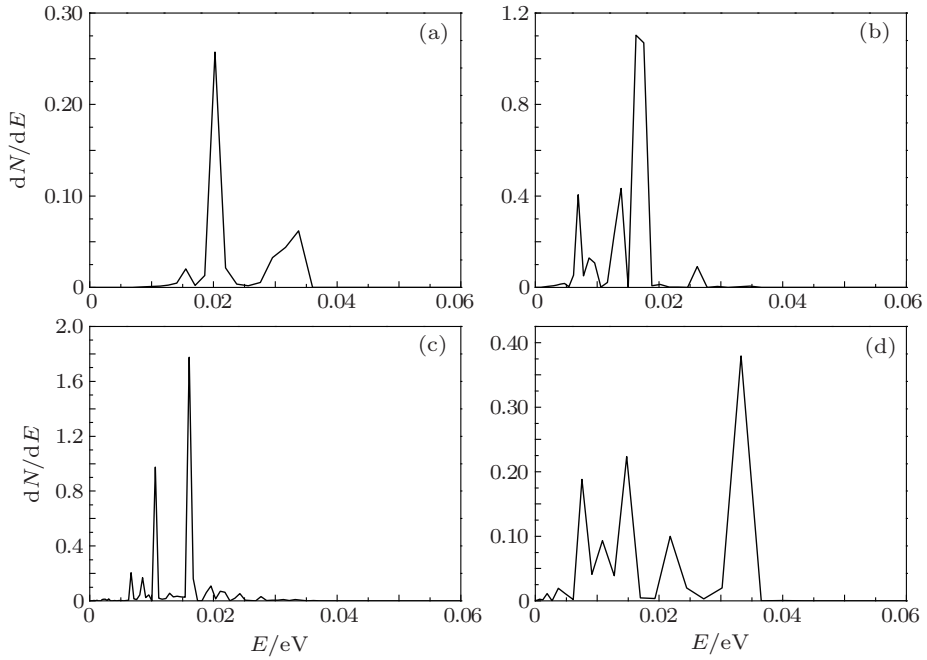


Fig. 4. Kinetic-energy distribution of dissociation fragments for laser intensities of (a) 8×10^{11} W/cm^2, (b) 8×10^{12} W/cm^2, (c) 8×10^{13} W/cm^2, (d) 8×10^{14} W/cm^2, in the lower channel.

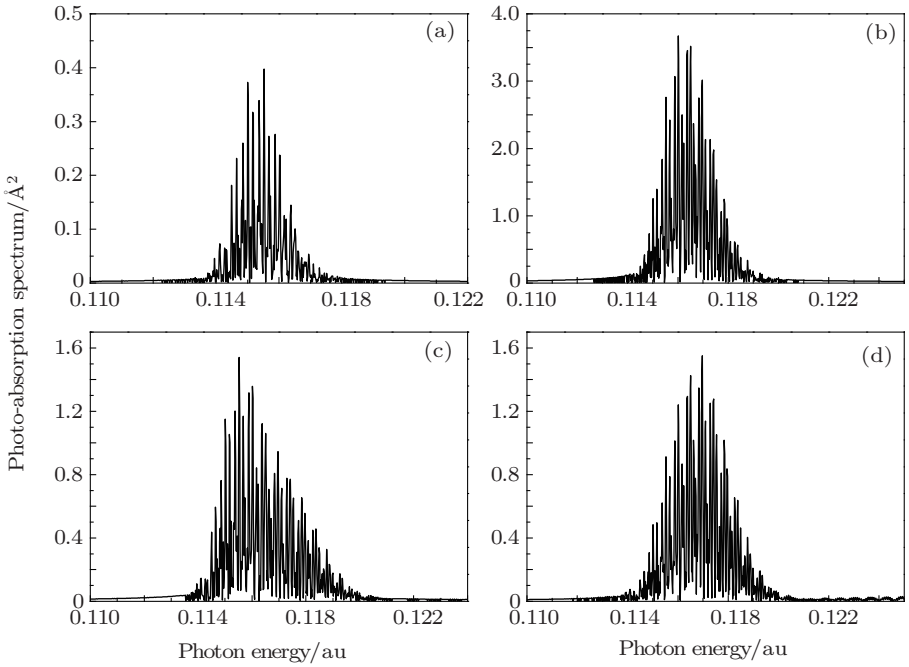


Fig. 5. Photo-absorption spectra in the lower channel at a wavelength of $\lambda = 400$ nm and different laser intensities: (a) 8×10^{11} W/cm^2, (b) 8×10^{12} W/cm^2, (c) 8×10^{13} W/cm^2, (d) 8×10^{14} W/cm^2.

The external field effect can be also shown in the photo-absorption spectrum. Generally the energy-dependent photo-absorption spectrum is simply the partial cross section, which is determined by the wave function in the energy domain (Eq. (15)). Figures 5 and 7 show, respectively, the photo-absorption spectra in the lower and upper channels at laser wavelength $\lambda = 400$ nm for different laser intensities. The height of the peak in the absorption spectrum corresponds to the population of each vibration level in the ground electronic state; the greater the population, the higher the peak is.[36] Since the excited-state covalent PECs are significantly modified by the field-molecule interaction, it is natural that the height of each spectrum peak changes with the external field. In other words, this influence ought to be exhibited in the absorption spectrum. From Fig. 5 one can find such a common feature that the broad envelope is superimposed with a series

of extremely narrow resonances separated by broad window resonances that recur periodically. This appearance can be attributed to the oscillation of the wave packet trapped in the well of the upper adiabat as mentioned before. As can be expected, the photon energy corresponding to the highest peak is the most probable energy with which the photon can be absorbed. It can also be observed from Fig. 5 that the bandwidth of the spectrum changes with laser intensity, too. This phenomenon can be explained by the fact that by increasing the laser intensity the photons with other frequencies have now enhanced probability to be absorbed in the photo-dissociation process. Inevitably when the laser intensity changes from 8×10^{11} Wcm^2 to 8×10^{12} W/cm^2 the band center displays a slight blue shift, while the laser intensity changing from 8×10^{12} W/cm^2 to 8×10^{13} W/cm^2 will lead to a slight red shift of the band center. The phenomenon that the band center changes with the increase of laser intensity can be explained by the fact that the coupling of the three electronic states by the external field may change the separation of the adjacent PECs in the Frank–Condon region. In order to verify the correctness of the absorption spectrum in Fig. 5, using the "Chebyshev polynomial expansion" scheme,[37] we calculate also the photo-absorption spectrum with only the ground state $X^1\Sigma^+$and the excited state $B^1\Sigma^+$ as shown in Fig. 6. Obviously the photon energy corresponding to the highest peak is also approximately equal to the difference between the minima of the two PECs which is exhibited in Fig. 1. The comparison of Fig. 5 with Fig. 6 shows that although they have the same band width, due to the existence of the avoided crossing and the external field, the PECs' shift will lead to the shift of the most probable energy, which cannot be found in Fig. 6. The difference between peak height in Fig. 5 and that in Fig. 6 can also be attributed to the couplings between the PECs and the external field. However because of the limitation of the "Chebyshev polynomial expansion" scheme, one cannot find the structure of the absorption spectrum in Fig. 6.

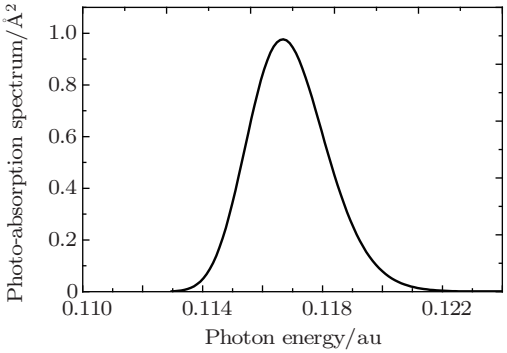


Fig. 6. Photo-absorption spectrum in the excited state $B^1\Sigma^+$ when only the ground state $X^1\Sigma^+$ and the excited state $B^1\Sigma^+$ exist.

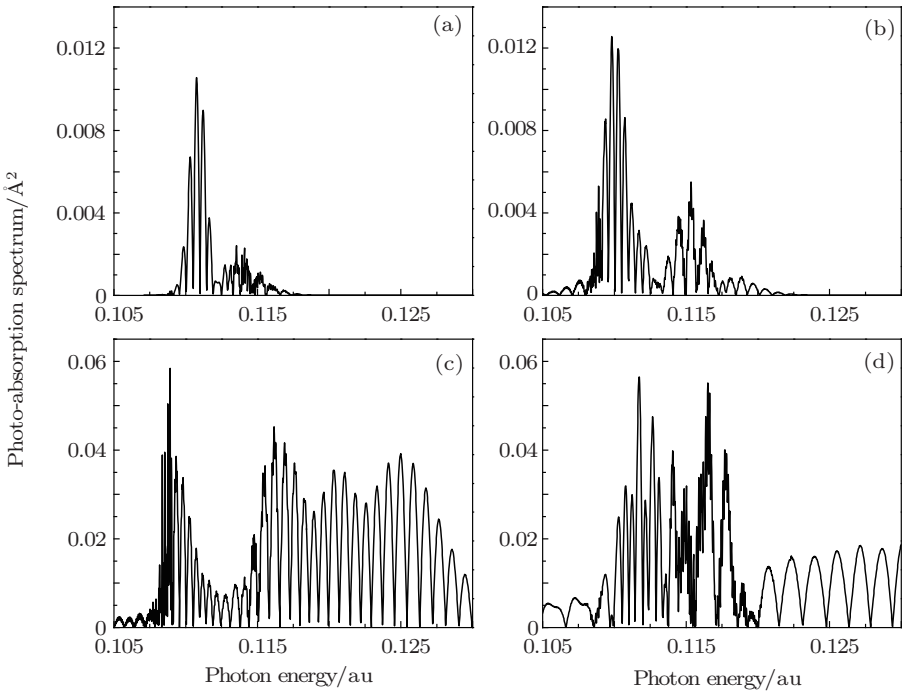


Fig. 7. Photo-absorption spectra in the upper channel at a wavelength of $\lambda = 400$ nm and different laser intensities: (a) 8×10^{11} W/cm^2, (b) 8×10^{12} W/cm^2, (c) 8×10^{13} W/cm^2, (d) 8×10^{14} W/cm^2).

From Fig. 7 we can see that there are almost no dissociation fragments through the upper channel, but due to the possibility to dissociate by the lower channel when they transmit the avoided crossing, there is still a certain absorption intensity. Unlike the photo-dissociation cross section in the lower channel, there is more than one envelope in the absorption spec-

trum of the upper channel. With the increase of laser intensity, the diffusion phenomenon of the absorption band seems to be more obvious. From the point of the spectrum, this diffusion of the absorption band arises from the existence of the predissociation limit. The existence of the predissociation limit causes the discrete energy levels to overlap with the continuous energy levels, giving rise to the non-radiative transition. If the transition probability between the electronic states is not unusually small, we can observe the diffusion of the absorption band, which is also the criterion of whether the predissociation limit exists. But the probability of non-radiative transition is not always too big to make the band completely diffuse, sometimes the individual spectral line has only a small broadening as shown in Figs. 7(a) and 7(b). When the laser intensity is increased, a notable broadening can be found in the absorption spectra as shown in Figs. 7(c) and 7(d). The change of the absorption spectrum with the laser intensity is related to the superposition of the wave packets and the influence of the external field on the potentials. As described in Section 2, the photo-absorption spectrum is determined by the wave function in energy (or time) domain. The increasing laser intensity leads to the changing of PECs, giving rise to the distortion of wave packets evolving on the PECs, and the superposition of the wave packets from the left- and right-hand-side turning points intensifies this distortion. This is the dynamic analysis for spectrum diffusion.

4. Conclusions

In this paper we use the TDWP method to investigate the photo-dissociation dynamics of NaCs. In order to achieve the influence of the external field on the dissociation dynamics, we examine the population of each state, photo-absorption spectra and dissociation kinetic-energy distributions changing with the external field. It is noticed that many interesting phenomena which occur in the photo-dissociation process are related to the avoided crossing of the two excited states and the predissociation limit. The results show that by increasing the laser intensity, the band center of the cross section in the lower channel has a shift. For the upper channel, because of the existence of the predissociation limit, we can find not only the diffusion of absorption bands, but also more than one envelope in the absorption spectrum. It should be noted that due to the modification of the PECs by the external field, the dissociation probability and the kinetic-energy distribution of the fragment also change with the increase of the laser intensity. These effects are very significant for understanding the external field manipulation of some chemical reaction processes. We hope that the present work can stimulate the future experimental investigations and have some significances for the production of the ultracold NaCs molecule.

References

[1] Butler L J and Neumark D M 1996 *J. Phys. Chem.* **100** 12801
[2] Lee S H 2010 *Phys. Chem. Chem. Phys.* **12** 2655
[3] Shapiro M, Hepburn J W and Brumer P 1988 *Chem. Phys. Lett.* **149** 451
[4] Charron E, Giusti-Suzor A and Mies F H 1993 *Phys. Rev. Lett.* **71** 692
[5] Sage J M, Sainis S, Bergeman T and DeMille D 2005 *Phys. Rev. Lett.* **94** 203001
[6] Zhang W, Xie T, Huang Y, Wang G R and Cong S L 2013 *Chin. Phys. B* **22** 013301
[7] Zhang C Z, Zheng B, Wang J and Meng Q T 2013 *Chin. Phys. B* **22** 023401
[8] Léonard C and Quéré F L 2012 *J. Chem. Phys.* **137** 164318
[9] Shi D H, Niu X H, Sun J F and Zhu Z L 2013 *J. Phys. Chem. A* **117** 2020
[10] Alekseyev A B, Liebermann H P, Buenker R J, Balakrishnan N, Sadeghpour H R, Cornett S T and Cavagnero M J 2000 *J. Chem. Phys.* **113** 1514
[11] Herzberg G 1983 *Molecular Spectra and Molecular Structure* (Beijing: Science Press) p. 307
[12] Grochola A, Szczepkowski J, Jastrzebski W and Kowalczyk P 2011 *J. Chem. Phys.* **135** 044318
[13] Kim J T, Lee Y, Kim B, Wang D J, Gould P L, Eyler E E and Stwalley W C 2012 *J. Chem. Phys.* **137** 244301
[14] Yu J, Shu C C, Hu W H and Cong S L 2010 *J. Theor. Comput. Chem.* **09** 785
[15] Jendoubi I, Berriche H, Ouada H Ben and Gadea F X 2012 *J. Phys. Chem. A* **116** 2945
[16] Yu J, Wang S M, Yuan K J and Cong S L 2006 *Chin. Phys.* **15** 1996
[17] Sharma A, Dixit M N and Bhale G L 1986 *J. Phys.* **27** 695
[18] Shen Y F and Li W X 2002 *Chin. J. Quantum. Electron.* **19** 410
[19] Aymar M and Dulieu O 2007 *Mol. Phys.* **105** 1733
[20] Lin F, Zhang W, Zhao Z Y and Cong S L 2012 *Chin. Phys. B* **21** 073203
[21] Zhao Z Y, Zhang W, Huang Y and Cong S L 2013 *Laser Phys.* **23** 035502
[22] Zhang H S, Ji Z H, Yuan J P, Zhao Y T, Ma J, Wang L R, Xiao L T and Jia S T 2011 *Chin. Phys. B* **20** 123702
[23] Meng Q T and Varandas A J C 2013 *Chin. Phys. B* **22** 073303
[24] Meng Q T, Yang G H, Sun H L, Han K L and Lou N Q 2003 *Phys. Rev. A* **67** 063202
[25] Wang J, Liu F, Yue D G, Zhao J, Xu Y, Meng Q T and Liu W K 2010 *Chin. Phys. B* **19** 123301
[26] Lu R F, Zhang P Y and Han K L 2008 *Phys. Rev. E* **77** 066701
[27] Yue D G, Zheng X Y, Liu H and Meng Q T 2009 *Chin. Phys. B* **18** 1479
[28] Paul A K, Adhikari S, Baer M and Baer R 2010 *Phys. Rev. A* **81** 013412
[29] Su Q Z, Yu J, Yuan K J and Cong S L 2012 *J. Theor. Comput. Chem.* **11** 709
[30] He H X, Lu R F, Zhang P Y, Han K L and He G Z 2012 *J. Chem. Phys.* **136** 024311
[31] Feit M D, Fleck J A and Steiger A 1982 *J. Comput. Phys.* **47** 412
[32] Neuhasuer D and Baer M 1989 *J. Chem. Phys.* **90** 4351
[33] Feuerstein B and Thumm U 2003 *Phys. Rev. A* **67** 043405
[34] Fererstein B and Thumm U 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** 707
[35] Meng Q T, Yang G H and Han K L 2003 *Int. J. Quantum. Chem.* **95** 30
[36] Han Y C 2009 "Theoretical Study of Ionization and Dissociation Dynamics of Diatomic Molecules in Femtosecond Laser Fields" (Ph. D. Dissertation) (Dalian: Dalian University of Technology) (in Chinese)
[37] Bhattacharjee A and Dastidar K R 2002 *Phys. Rev. A* **65** 022701