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Interference effects on the photoionization cross sections between two neighbouring atoms: nitrogen as an example*

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Interference effects on the photoionization cross sections between two neighbouring atoms are considered based on the coherent scattering of the ionized electrons by the two nuclei when their separation is less than or comparable to the de Broglie wave length of the ionized electrons. As an example, the single atomic nitrogen ionization cross section and the total cross sections of two nitrogen atoms with coherently added photoionization amplitudes are calculated from the threshold to about 60 Å (1 Å=0.1 nm) of the photon energy. The photoionization cross sections of atomic nitrogen are obtained by using the close-coupling *R*-matrix method. In the calculation 19 states are included. The ionization energy of the atomic nitrogen and the photoionization cross sections agree well with the experimental results. Based on the *R*-matrix results of atomic nitrogen, the interference effects between two neighbouring nitrogen atoms are obtained. It is shown that the interference effects are considerable when electrons are ionized just above the threshold, even for the separations between the two atoms are larger than two times of the bond length of N_2 molecules. Therefore, in hot and dense samples, effects caused by the coherent interference between the neighbours are expected to be observable for the total photoionization cross sections.

Keywords: interference effect, photoionization cross section, nitrogen atom

PACC: 3280F, 4210J, 3120A

1. Introduction

When an electron is elastically scattered by two neighbouring atoms, as described by Messiah,[1] the elastic scattering amplitudes caused by these two atoms may add coherently, resulting in interference effects on the scattering cross sections. These interference effects may also happen during the photoionization process of a diatomic molecule, such as molecular hydrogen, which was first studied by Cohen and Fano[2] decades ago. Such an electron emission from H_2 is similar to the Young's two-slit experiment, which played an important role during the development of the quantum mechanics. From then on, both theoretical and experimental physicists showed great interests on such interference effects. For different impact objects, interference effects from collision photoionization cross section of H_2 and D_2 were studied.[3−8] Nage *et al*[6] studied the interference effects in the photoionization of molecular hydrogen by using random phase approximation. In 2007, Fernández *et al*[8] presented a theoretical study on fast-electron photoionization of H_2 and H_2^+. In their paper, the typical Young's two-slit interferences were found when the molecules oriented perpendicularly to the polarization direction of the light. But only very recently, has the interference effects been observed in the experiments[9−12] of electron emission from H_2 collision with heavy ions. For nitrogen molecule, Samson *et al*[13] measured the total and dissociative photoionization cross section from its threshold to 107 eV. At higher photon energy, the cross sections are almost twice that of the atomic nitrogen, but not at the lower photon energy. However, the inner shell 1s electron photoionization gives a different picture. Rolles *et al*[14] observed the coherence of core electrons in N_2 through a direct measurement of the interference exhibited in their emission and also explored isotope-induced partial localization of core electrons in the homonuclear N_2. Liu *et al*[15,16] revised Cohen–Fano's two-centre interference phenomenon using core-level photoemission from N_2. By using an Auger electron angular emission patterns from molecular nitrogen after inner-shell ionization as an ultrafast probe of hole localization, Schöffler *et al*[17] claimed that they can clarify whether the core

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vacancy created in a homonuclear diatomic molecule is localized on one atom or delocalized over both. In molecular bonding frameworks, the valence electrons are clearly delocalized, that is why the valence electron photoionization cross sections of molecular nitrogen do not show an interference pattern.[13] But when two nitrogen atoms are not so close as to form a molecule and also not so far as to be treated as two independent atoms as people often met in hot and dense gases or plasmas,[18−20] the interference effects should occur.

The total photoionization cross sections of atomic nitrogen are important both in probing the details of atomic structure and in the understanding of gaseous discharges, stellar atmosphere and solar-terrestrial effects. So the photoionization cross sections of nitrogen atoms are of interest to both theoretical and experimental studies. From Bates and Seaton,[21] using the Hartree–Fock approximation, many other theoretical calculations have been done.[22−28] Henry[22,23] considered the dipole length and velocity approximation and then included the effects of coupling between final-state channels to obtain the photoionization cross section of atomic nitrogen. Other methods such as the central potential method,[24] the scaled Thomas–Fermi method[25,26] and the independent-particle model[27] have also been used to predict the photoionization cross section of atomic nitrogen. Le Dourneuf *et al*[28] used the R-matrix method to give the photoionization cross sections of atomic nitrogen from the threshold to 3 Ryd. In their R-matrix calculation, single excitations to 3s, 3p and 3d pseudo-orbitals were included for electron correlation effects. On experiments side, because of the difficulty in producing a sufficient number of free atoms from the dissociation of N_2, only a few experimental studies on the photoionization cross sections have been made.[29−31] Ehler and Weissler[29] reported the first measurement of the absolute absorption cross sections between 400 Å and 700 Å. Comes and Elzer.[30] reported the cross sections over the range 450–852 Å later. Samson and Angel[31] carried out independent measurements of the absolute photoionization cross section from the threshold to 31 Å. Dehmer *et al*[32] measured the relative cross section for atomic nitrogen from 870 Å to 600 Å at a wavelength resolution of full width at half maximum (FWHM) equal to 0.83 Å. Five members of the autoionizing Rydberg series $2s2p^3(^5S^o)np^4P$ were observed in their experiment. Though the existing experimental and theoretical results agree with each other in shape, the discrepancies at relatively lower energy cannot be ignored. From the threshold to about 500 Å, the theoretical predictions are higher than experimental results. More accurate theoretical study is necessary.

In the present study, the photoionization cross section of atomic nitrogen will be obtained by using the close-coupling R-matrix method with photon energies from threshold to about 60 Å. In the calculation, more single orbitals will be used in the close coupling expansion and the core-valence (CV) electron interaction will be included. Further investigation is focused on the interference effects which may occur between the two nearby nitrogen atoms during the photoionization process.

2. Theoretical methods

The R-matrix method for electron–atom and photon–atom interactions has been discussed in great detail by Burke *et al*.[33] The present calculations have been carried out by using the Belfast atomic R-matrix code.[34] We will just give an outline as follows.

In an R-matrix calculation, the wave function of the N+1 electron system is given by the form

$$\Psi_k(X_1 \dots X_{N+1}) = \hat{A} \sum_{ij} c_{ijk} \phi_i(X_1 \dots X_N; \hat{r}_{N+1}\sigma_{N+1}) \times u_{ij}(r_{N+1}) + \sum_j d_{jk} \Phi_j(X_1 \dots X_{N+1}), \qquad (1)$$

where $\hat{A}$ is the antisymmetrization operator to take the exchange effects between the target electrons and the free electron into account. X_i stands for the spatial (r_i) and the spin (σ_i) coordinates of the i-th electron. The functions $u_{ij}(r)$ under the first sum construct the basis sets for the continuum wavefunctions of the free electron. For each angular momentum, they are obtained by solving the model single-channel scattering problem and are orthogonal both to themselves and to the bound orbitals. The bound orbitals plus the continuum orbitals then form a much larger size of basis set for the N+1 electron system than that for the N electron target states. Φ_i is the coupling between the target wavefunction of a specific level and

the angular and spin part of the free electron. The target states are usually written as a configuration-interaction (CI) expansion in terms of some basis configurations, which are constructed from a bound orbital basis set consisting of self-consistent field orbitals plus some additional pseudo-orbitals to model electron correlation. The correlation functions ϕ_j in the second sum are formed from the same set of bound orbitals and must be included to compensate for the incompleteness of the continuum orbitals. They can also be used to compensate for the correlation effects not adequately considered because of the cut-off in the first sum. The square integrable orbitals are cast as linear combinations of Slater-type orbitals

$$P_{nl} = \sum_j C_{jnl} r^{I_{jnl}} \exp(-\xi_{jnl} r), \qquad (2)$$

in which the number of Slater-type orbitals, necessary to sufficiently approximate these orbitals P_{nl}, increases as the number of spherical nodes of P_{nl} becomes larger.

In the present calculation, 10 single electron orbitals are included to form the configuration interaction wavefunction of the positive nitrogen. The pertinent parameters ξ_{jnl} and coefficients C_{jnl} for 1s, 2s, and 2p are the same as those of the Hartree–Fock orbitals given by Clementi and Roetti[35] for the N^+ ($1s^2 2s^2 2p^2\ ^3P$) state. The 3s, 3p, and 3d orbitals are spectroscopic and optimized on the $2s^2 2p3s\ ^3P^o$, $2s^2 2p3p\ ^3P$, and $2s^2 2p3d\ ^3P^o$ states, respectively, while the 4s, 4p, 4d, and 4f are optimized on the three lowest levels of the positive nitrogen by using the structure code CIV3.[36] Same as the oxygen photodetachment process[37] we have studied before, the core-valence (CV) electron interaction is also found to be important in the present calculation. After considering the excitation of the two 2s electrons to higher electron orbitals with 1461 configurations in total, the calculated energy levels of the positive nitrogen agree with the experimental results[38] fairly well. The energy levels of the lowest 19 states for the positive nitrogen, which are included in the close-coupling, relative to the ground state are shown in Table 1 together with the experimental results.[38] From Table 1 one can see that the differences between the theoretical and experimental results are within 2%. On the other hand, the first ionization energy of the atomic nitrogen is important because it gives the position of the threshold of the photoionization cross section. In the present calculation, the first ionization energy increases due to the contribution of the so-called CV electron correlation, the same as the oxygen photodetachment process,[37] where the inclusion of CV correlation increases the electron affinity. The present calculated first ionization energy of 14.502 eV is very close to the experimental value of 14.534 eV.[39] The agreements of the energy levels and the first ionization energy between the present calculation and the experimental results make us believe that the wavefunction of the positive nitrogen for the present photoionization calculation is reliable.

Table 1. Calculated energy levels (in eV) of the first 19 low-lying excited states of positive nitrogen compared with experimental results.[38] ΔE is the absolute difference between calculation and experiment (relative differences are given in the parenthesis).

state	present	expt.	ΔE
$2s^2 2p^2\ ^3P$	0.000	0.000	0.000
$2s^2 2p^2\ ^1D$	1.938	1.899	0.039 (2.1%)
$2s^2 2p^2\ ^3D$	4.101	4.053	0.048 (1.2%)
$2s2p^3\ ^5S^o$	5.607	5.801	–0.194 (–3.4%)
$2s2p^3\ ^3D^o$	11.463	11.437	0.026 (0.2%)
$2s2p^3\ ^3P^o$	13.626	13.541	0.085 (0.6%)
$2s2p^3\ ^1D^o$	18.185	17.877	0.308 (1.7%)
$2s^2 2p3s\ ^3P^o$	18.765	18.473	0.293 (1.6%)
$2s^2 2p3s\ ^1P^o$	18.795	18.497	0.298 (1.6%)
$2s2p^3\ ^3S^o$	19.468	19.233	0.235 (1.2%)
$2s^2 2p3p\ ^1P$	20.744	20.409	0.335 (1.6%)
in $2s^2 2p3p\ ^3D$	20.970	20.658	0.312 (1.5%)
$2s2p^3\ ^1P^o$	21.039	20.676	0.363 (1.8%)
$2s^2 2p3p\ ^3S$	21.210	20.940	0.270 (1.3%)
$2s^2 2p3p\ ^3P$	21.427	21.154	0.273 (1.3%)
$2s^2 2p3p\ ^1D$	21.886	21.560	0.326 (1.5%)
$2s^2 2p3p\ ^1S$	22.458	22.103	0.355 (1.6%)
$2s^2 2p3d\ ^3F^o$	23.436	23.135	0.301 (1.3%)
$2s^2 2p3d\ ^1D^o$	23.520	23.196	0.324 (1.4%)

When there are two of the same kinds of atoms close to each other, during the single photoionization process, the interference effects may occur. To investigate the interference effects, we apply a formalism analogous to that developed for electron elastic scattering from two atoms,[1] which had also been discussed by Stolterfoht *et al.*[9] Atomic units are used throughout if not otherwise stated. The photoionization cross section from two atoms can be written as

$$\frac{\mathrm{d}\sigma_{N-N}}{\mathrm{d}\Omega \mathrm{d}\epsilon \mathrm{d}\boldsymbol{k}} = \frac{\mathrm{d}\sigma_{2N}}{\mathrm{d}\Omega \mathrm{d}\epsilon \mathrm{d}\boldsymbol{k}} [1 + \cos(\boldsymbol{k}\cdot\boldsymbol{d})], \qquad (3)$$

where the cross section $\mathrm{d}\sigma_{N-N}/\mathrm{d}\Omega \mathrm{d}\epsilon \mathrm{d}\boldsymbol{k}$ describes the photoionization cross section from the two atoms separated by $\boldsymbol{d}$, while the cross section $\mathrm{d}\sigma_{2N}/\mathrm{d}\Omega \mathrm{d}\epsilon \mathrm{d}\boldsymbol{k}$ refers to that of two atoms acting as independent particles. The solid angle $\mathrm{d}\Omega$ and the energy $\mathrm{d}\epsilon$ refer to

the outgoing electron. The vector $\boldsymbol{k}$ is the momentum of the ionized electron, while $\boldsymbol{d}$ is the vector associated with the internuclear distance of the two atoms. After performing an average over the orientation of the internuclear axis of the two neighbouring atoms, we obtain the relationship

$$\frac{\mathrm{d}\sigma_{N-N}}{\mathrm{d}\Omega \mathrm{d}\epsilon \mathrm{d}\boldsymbol{k}} = \frac{\mathrm{d}\sigma_{2N}}{\mathrm{d}\Omega \mathrm{d}\epsilon \mathrm{d}\boldsymbol{k}} \left[1 + \frac{\sin(kd)}{kd}\right]. \qquad (4)$$

The term in the parenthesis represents the interference caused by the two neighbouring atoms.

3. Results and discussion

3.1. Calculated photoionization cross section of single nitrogen atom

First, the photoionization cross sections from the threshold to 60 Å are obtained, as shown in Fig.1 together with the experimental results.[31] The solid line stands for the length form of the photoionization cross section, while the long-dashed line for the velocity form. The empty circles are the experimental results.[31] The present cross sections are the convolution integral of the R-matrix results with a Gaussian function, which is due to the resolution of 0.6 Å of the experimental instruments.[40] One can find that the calculated length and velocity forms of the cross section agree with each other fairly well and also agree with the experimental results well in shape. From the threshold to about 570 Å, the theoretical photoionization cross sections are higher than the experimental results.[31] The present results are similar to those of a former R-matrix results,[28] not plotted in Fig.1 for the clarity of the figure. As the agreement between independent calculations is very good, the systematic discrepancies between theory and experiment are most likely due to experimental uncertainties. As an example, a gradually overestimation of the excitation laser intensities with the wavelength may induce underestimated photoionization cross sections from higher photon energies to the photoionization threshold. The present results also predict the $2s2p^3(^5S^o)np$ Rydberg series from the threshold to about 600 Å, which are marked in Fig.1. These autoionization resonances were observed first by Carroll *et al*[41] and later by Dehmer *et al*[32] and had been investigated by Smith and Ormonde[42] using the multiconfiguration close-coupling method. It can be explained as follows. When the photon energy E is higher than the first ionization energy, i.e., 14.502 eV in the present calculation, one of the 2p electrons is ionized to be free electron with energy of (E-14.502) eV. As the photon energy increases, the independent particle model would predict the existence of two conflicting atomic terms: firstly, it would predict a continuum term ψ with configuration $2s^22p^2$ (kL) ^{4}P, with L referring to s-electron or d-electron; secondly, it would predict a stationary eigenstate ϕ with configuration $2s2p^3(^5S^o)np$ ^{4}P ($n \geq 2$). However, the continuum term and the stationary eigenstate should be superimposed in order to give a more accurate theoretical description of the system. Actually, one can envisage this coupling of the two independent particle configurations as providing a mechanism for the discrete ϕ to dissociate into an electron and an N^+ ion. This autoionization phenomenon can be understood as that when one of the 2p electrons decays to 2s orbital, it provides energy for releasing the np electron into the continuum. A detailed comparison of the autoionizing Rydberg state $2s2p^3(^5S^o)3p$ between the present results and the experimental results of Dehmer *et al*[32] is shown in Fig.2. In the figure, the solid and dotted lines are the present length and velocity form cross section convoluted with the Gaussian instrumental function with the FWHM of 0.83 Å. Our results have been moved 0.2 eV to higher photon energy. The long dashed line is the Fano profile after convolution. The two symbols, cross and empty circles, refer to two different scans over the line in the experiment. Since the experimental results

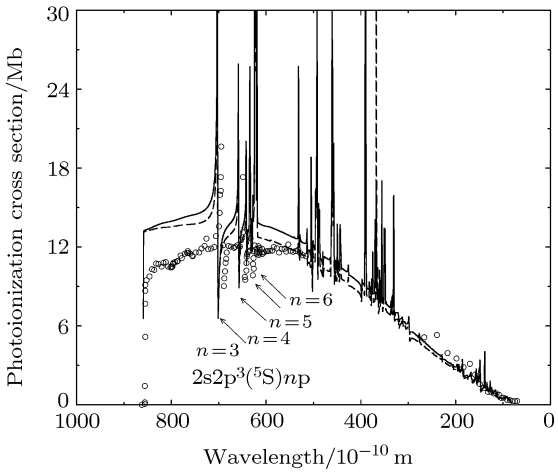


Fig.1. The total photoionization cross sections of atomic nitrogen. The solid line is the length-form result, and the long dashed line is the velocity-form result. The empty circles are experimental results.[31]

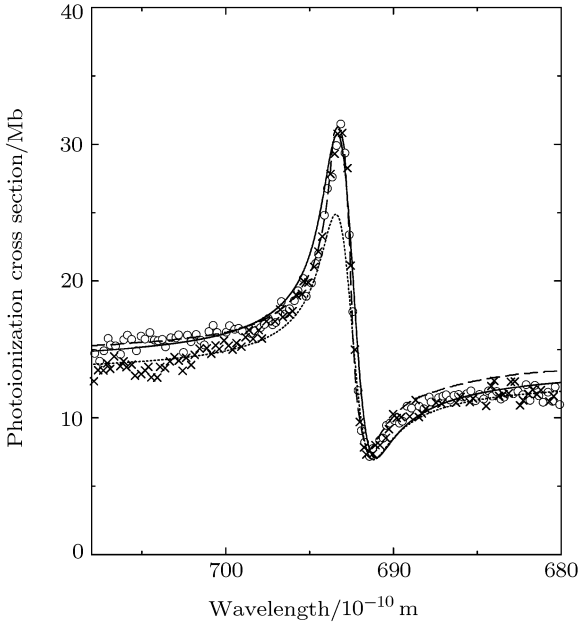


Fig.2. The autoionizing resonance from the Rydberg state $2s2p^3(^5S^o)3p$. The solid and dotted lines are the present length and velocity forms of photoionization cross section. The long dashed line is the Fano profile.[32] The empty circles and crosses are two different scans over the line in the experiment.[32]

are relative cross section, we normalize the peak of the experimental results to our cross section in length-form. One can find that after fitting, the theoretical length form cross sections agree with the experimental results perfectly. The 10% discrepancy between the length and velocity form of the R-matrix results are reasonable.

The contributions of the individual ionization channels to the total cross section are also obtained in the calculation. When the photon energy reaches 14.502 eV, the $2s^22p^2\ ^3P$ channel opens and the nitrogen atom is ionized. As the photon energy increases further, the autoionization resonances occur. When the photon energy reaches the point equal to the first ionization energy plus the energy of transition from ground state positive nitrogen to the excited state $2s2p^3$, the $2s2p^3\ ^5S^o$ channel opens. More and more channels open as the photon energy is getting higher and higher. The cross section of the first four channels are given in Fig.3. The solid lines stand for the length form of the cross section, while the long dashed lines for the velocity form.

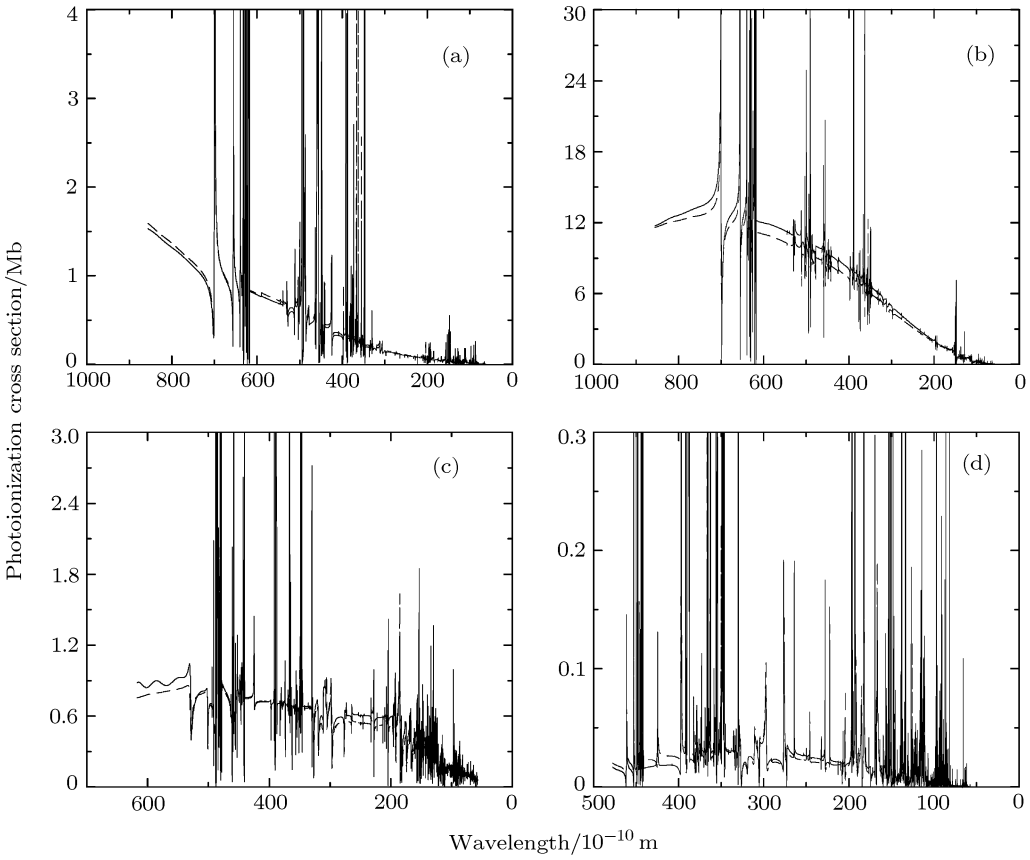


Fig.3. Contributions from first four individual ionization channels. The solid and long dashed lines are the length and velocity form photoionization cross sections. (a), (b), (c), and (d) refer to contributions from $2s^22P^2$ 3P+ks, $2s^22p^2$ 3P+kd, $2s2p^3\ ^5S^o$+kp, and $2s2p^3\ ^3P^o$+kp channels respectively.

Figure 3(a) shows the contribution from $2s^22p^2\ ^3P$+ks channel. From the threshold one can see typical *s*-electron scattering shape. Figure 3(b) gives the contribution from $2s^22p^2\ ^3P$+kd channel. The absolute photoionization cross section shows that the $2s^22p^2\ ^3P$+kd channel contributes most to the total cross section. Figure 3(c) and 3(d) are contributions from $2s2p^3\ ^5S^o$+kp and $2s2p^3\ ^3P^o$+kp channels respectively. The contributions from other individual ionization channels are small and not shown in the figure.

3.2. Interference effects on the total photoionization cross sections of two closely neighbouring nitrogen atoms

Based on the present photoionization cross section of the nitrogen atom, we investigate the cross section from two nitrogen atoms close to each other. Figure 4 gives half of the total integral photoionization cross section of two neighbouring nitrogen atoms obtained by integrating Eq.(4) over outgoing electron angles with a few different interatomic distances. The photoionization cross section of a single nitrogen atom is also shown in the figure for comparison. Only the length form of the cross sections is shown in the figures. The solid lines are half of the cross section with interference effects between two neighbouring nitrogen atoms, while the long dashed lines are the present *R*-matrix results for single nitrogen atom. One can see from the figures that as the distances between two nitrogen atoms are different, the shapes of the total cross section are different. Near the threshold, the closer the two nitrogen atoms, the bigger the differences between the interference results and the single atom photoionization results. When the energy of the outgoing electron is high enough, the interference effects vanish. It can be understood that when the energy of the outgoing electron gets higher, the de Broglie wave of the electron becomes shorter, same as the results in Young's two-slit experiment, the interference effects cannot be observed. In Fig.4(a), the distance between two nitrogen atoms is 2 a.u., almost the same as the nuclear distance of the two atoms in the molecular nitrogen.

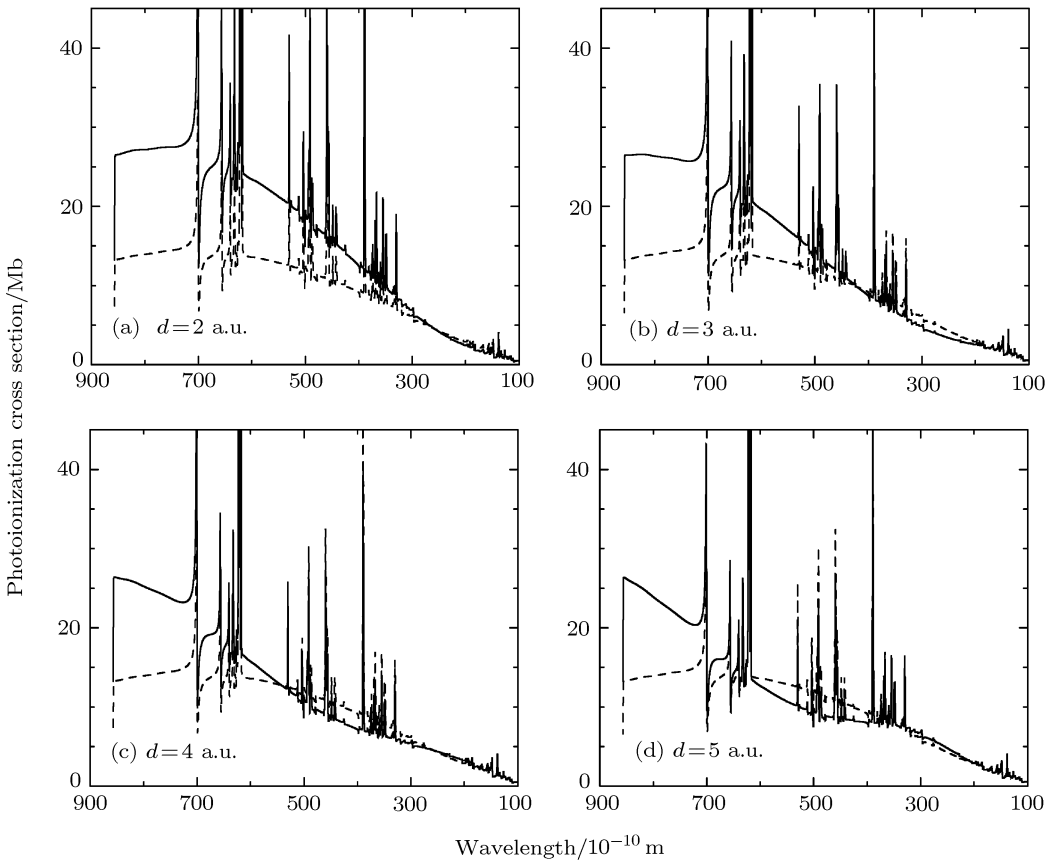


Fig.4. Half of the total integral photoionization cross sections with different distances between two neighbouring nitrogen atoms. The solid lines are cross sections from two neighbouring nitrogen atoms and the long dashed lines are the *R*-matrix results. (a)–(d) refer to the results with d = 2, 3, 4 and 5 a.u. respectively.

It is not surprising that the results obtained with interference effects differ from the photoionization cross section of N_2 observed by Samson *et al.*[13] As we have mentioned before, when two nitrogen atoms form a molecular nitrogen, the valence electron of the atoms is delocalized, thus the photoionization cross section cannot be interpreted by the two centre interference effects. But when the distance of the two nitrogen atoms is not so close as to form a bonding, the interference effect should be observed in the photoionization cross section. For different energies of the outgoing electron, from Fig.5(a)–5(d), half of the photoionization cross section in length form along with the nuclear distance of the two nitrogen atoms are shown. At photoelectron energies of 0.1, 0.5, 1, and 3 a.u., the R-matrix results are 15.0579, 12.3296, 6.0795 and 1.0881 Mb, respectively. From Fig.5 one can find that at energy of the outgoing electron of 0.1 and 0.5 a.u., the interference results are almost twice that of the R-matrix results while vary relatively slow. When the energy of the outgoing electron is 3 a.u., the cross section does not change

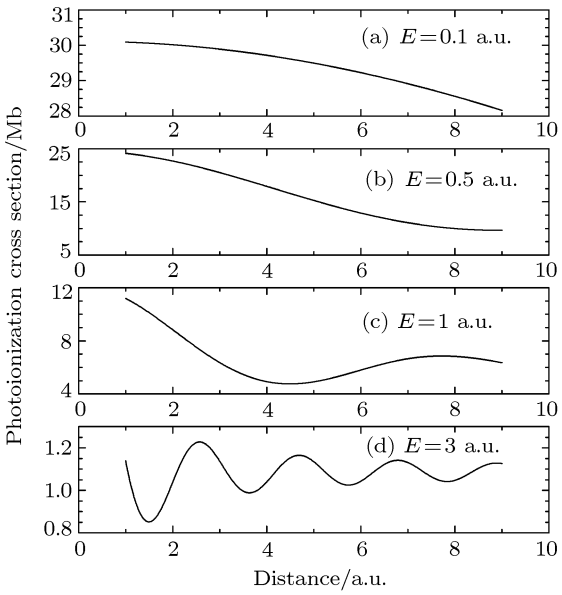


Fig.5. Half of the photoionization cross sections with the nuclear distances of two nitrogen atoms at photoelectron energies of 0.1, 0.5, 1, and 3 a.u. respectively.

very much but oscillates quickly and the interference effects are obvious. Though there are no experimental results to directly prove the present prediction, the interference effects should not be ignored in some circumstances when two particles are not so close to form a bonding, but also not so far away to be treated as independent particles. The near threshold photoionization absorption is often used to diagnose the energy level and ion populations in a hot and dense plasmas,[43] and the understanding of the coherent interference effects on the near threshold photoionization cross sections is essential for us to gain accurate answers. After one obtains the distribution of the distances between the atoms in a hot and dense sample by using statistical methods,[44] the average interference effects on the effective radiative absorptions or opacities can be evaluated with the present scheme. Further work are undergoing to study the photoionization process in hot and dense plasmas.

4. Conclusion

In conclusion, the interference effects on the photoionization process have been studied when two nitrogen atoms are close to each other. It is found that when the two atoms form a molecular nitrogen, the photoionization cross sections of N_2 cannot be interpreted by the interference effects. When the nuclear distances of the two nitrogen atoms get bigger and they cannot form a bonding, the interference effects are obvious. On the other hand, when the energy of the outgoing electron is small, the photoionization cross sections change a lot, comparable to twice the single nitrogen photoionization cross section. As the energy of the outgoing electron increases, the cross section oscillates quickly because of the interference effect. The photoionization cross sections of a single nitrogen atom are obtained by using the close coupling R-matrix method. The present results agree with the experimental results fairly well, and further investigation finds that the photoionization cross sections are mostly attributed to the $2s^22p^2$ 3P+kd individual ionization channel. We also predict the autoionizing Rydberg series $2s2p^3(^5S^o)np\ ^4P$ and make a thorough comparison with the experimental results for the $2s2p^3(^5S^o)3p\ ^4P$ autoionization resonance.[32] By moving 0.2 eV to a higher photon energy, our prediction on the $2s2p^3(^5S^o)3p\ ^4P$ autoionization resonance agrees with the experimental results perfectly.

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