Vol 17 No 10, October 2008
1674-1056/2008/17(10)/3649-06

Chinese Physics B

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The differential interference angle of $^2\Pi$[Case(a)] diatom on rotational energy transfer in NO($X^2\Pi$) collision with He, Ne and Ar system*

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(Received 23 October 2007; revised manuscript received 26 May 2008)

To study theoretically the relationship between the differential interference angle and the scattering angle in collisional quantum interference (CQI), we have investigated the differential interference angle of the atom–diatomic [case(a)] molecule system in detail. For the $^2\Pi$ electronic state in Hund's case (a), the degree of the differential interference is also discussed. The differential interference angles of NO($X^2\Pi$) are calculated quantitatively for the rotational energy transfer in Hund's case (a) induced by collision with He, Ne and Ar atoms. The method to calculate the differential interference angle is presented. Several factors that affect the differential interference angle are investigated. Finally the variation of the differential interference angle with the impact parameter and relative velocity is discussed.

Keywords: collisional quantum interference, rotational energy transfer, interference angle, long-range interaction potential

PACC: 3000, 3400

1. Introduction

Quantum interference (QI) in chemical dynamics is one of the main subjects in experiment and theory.[1−17] Experimentally, the QI was used in study on rotational energy transfer, decay, photodissociation, reaction scattering, and spectroscopy. A variety of modern experimental techniques have been employed for investigating collision-induced rotational energy transfer of diatomic molecules in Π electronic states.[18−22] In the open-shell Π-states, the collisional quantum interference(CQI) in rotational energy transfer has been observed experimentally, which results from the Λ splits of open-shell Π-states diatomic molecules, such as the Π-state alkali dimers Li_2 ($B^1\Pi_u$), Na_2, NaLi ($^1\Pi$) experiments: rotationally inelastic collisions of AIH ($A^1\Pi$) with Ar, rotational energy transfer of CO ($A^1\Pi$, $v = 3$) induced by collision with He, Ne and Ar atoms, and the rotational inelastic scattering for NO by Ar. The CQI in intermolecular rotational energy transfer was obtained by Sha *et al*[1−5] in the CO A1$\Pi(v = 0) \sim e^3\Sigma^-(v = 1)$ system in collision with He, Ne and other partners. CQI was also observed by Chen *et al*[6] in Na_2A $^1\Sigma_u^+(v = 8) \sim b^3\Pi_{0u}(v = 14)$ system in collision with Na (3s).

Theoretically, the interference effects on several collision systems are also discovered and discussed such as NO($X^2\Pi$)+Ar,[23−27] OH($X^2\Pi$)+ Ar,[28] CN($A^2\Pi$)+Ar[29] and CN($X^2\Sigma^+$, $A^2\Pi$)+Ar.[30] Maricq[31] presented his calculations for the oscillation distribution of cross sections within the systems Li_2, Na_2, N^2+ and CN in collision with rare gases. Dagdigian[32] and Alexander[33] studied the interaction potential for the interaction of a closed-shell atom with a molecule in an electronic state of $^2\Pi$-symmetry.

The theoretical explanation of the above experiments was given in Refs.[7]–[16], and the calculated results were consistent with the experimental results. The interference angles of rotational energy transfer of NO($X^2\Pi$) in Hund's case (a)

*Project supported by the National Natural Science Foundation of China (Grant No 10374040) and the Fund of the Educational Department of Liaoning Province, China (Grant No 20060347).
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induced by collision with He, Ne and Ar atoms were calculated quantitatively.[17] A dynamic model of atom-$^2\Pi$[case(a)] diatomic molecules system was reported.[7] As the further theoretical study on the collision-induced Λ-related quantum interference in rotational energy transfer in an atom-$^2\Pi$[case(a)] diatomic molecules system, the differential interference angles which reflect the degree of quantum interference (resulting from the Λ splits) are calculated. For the $^2\Pi$ electronic state in the Hund's case (a), the variation trend of differential interference angle of NO($X^2\Pi$) colliding with He, Ne and Ar atoms is discussed. This model can be used in the simulation of molecular beam experiments for calculating differential cross sections and differential interference angle.

2. Theoretical approach

For an atom–diatom system, the interaction potential V can be written as[34]

$$V(R,\theta,\phi)=\sum_{l,m,k} V_{l,k}(R)D^{l}_{m,k}(\Omega)\,C^{l}_{m}(\theta,\phi), \quad (1)$$

where R is the orientation from the atom to the mass centre of the diatom, $D^{l}_{m,k}(\Omega)$ is the Wigner D rotational matrix; the Euler angles $\Omega=\alpha,\ \beta,\ \gamma$ refer to the space fixed by the orientation of the diatom, $C^{l}_{m}(\theta,\ \phi)$ is a Racah spherical harmonic function, the angles θ and ϕ describe the orientation of R in the space frame. In the atom and $^1\Pi$-state diatomic molecules system, we have $k=0$ or $k=\pm2$.[32] The evolution of the interaction potential is

$$V(t)=U^{+}(t,0)VU(t,0), \quad (2)$$

where $U(t,0)$ is the time evolution operator,

$$U(t,0)=\exp(-\mathrm{i}H_0t/\hbar). \quad (3)$$

For the $^2\Pi$ electronic state in Hund's case (a), wavefunctions are of definite parity and may be written as[33]

$$\left|JM^2\Pi_{\Omega\varepsilon}\right\rangle=\frac{1}{\sqrt{2}}\Big[\left|JM\Omega\right\rangle\left|\Lambda=1,\ \Sigma=\pm1/2\right\rangle + \varepsilon\left|JM,-\Omega\right\rangle\left|\Lambda=-1,\ \Sigma=\mp1/2\right\rangle\Big], \quad (4)$$

where J is the total angular momentum quantum number, M is the projection of J along a space-fixed Z-axis, $\varepsilon=\pm1$. The parameter ε will be designated as the parity index. Within the spectroscopic nomenclature, the $\varepsilon=+1$ levels are designated as e and the $\varepsilon=-1$ levels as f. The wavefunction given in Eq.(4) is a correct description of a molecule in a $^2\Pi$ electronic state, only when the magnitude of the spin-orbit constant A is infinitely large compared to the product of the rotational constant B and the total angular momentum quantum number J. The rotational wavefunction $|JM\Omega\rangle$ which appears in Eq.(4) can be written as a rotational matrix element, namely,

$$\left|JM\Omega\right\rangle=\left[(2J+1)/8\pi^2\right]^{1/2}D^{J*}_{M\Omega}(\alpha\beta\gamma). \quad (5)$$

Considering the interaction between a $^2\Pi$[case(a)] diatom and a spherical atom in a singlet state, the total wavefunction is usually expanded in terms of eigenfunctions of the total angular momentum $\Im$, which is defined as[32]

$$\left|J\Omega\varepsilon\Im\varsigma\right\rangle=\sum_{MM_L}\left\langle JMLM_L|\Im\varsigma\right\rangle\left|LM_L\right\rangle\left|JM\varepsilon\right\rangle, \quad (6)$$

where ς is the space-frame projection of $\Im$, L is the orbital angular momentum of the atom-molecule pair with space-frame projection, and $|LM_L\rangle$ is a spherical harmonic,[33]

$$\left|LM_L\right\rangle=Y^{L}_{M_L}(\theta,\phi)=\left[(2L+1)/4\pi\right]^{1/2}D^{L}_{M_L,0}(\theta,\phi,0). \quad (7)$$

According to the first-order Born approximation, by taking into consideration of the product of three rotation matrix elements and spherical harmonics, and the relationship between $3j$ symbol and $6j$ symbol, the transition matrix element is expressed as[19]

$$\begin{aligned}&\left\langle J'L'\varepsilon'^2\Pi'_{\Omega}\Im\varsigma\right|V(t)\left|JL\varepsilon^2\Pi_{\Omega}\Im\varsigma\right\rangle\\ =&(-1)^{J+J'+\Im-\Omega}[(2J+1)(2J'+1)(2L+1)(2L'+1)]^{1/2}\sum_{l}\frac{1}{2}[1-\varepsilon\varepsilon'(-1)^{J+J'+l}]\times\begin{pmatrix}L' & l & L\\ 0 & 0 & 0\end{pmatrix}\begin{Bmatrix}J & L & \Im\\ L' & J' & l\end{Bmatrix}\\ &\times\left\{\delta_{\Omega\Omega'}\begin{pmatrix}J' & l & J\\ -\Omega' & 0 & \Omega\end{pmatrix}\exp(\mathrm{i}\varpi^{\Delta\Omega=0}_{J'J}t)V_{l,0}[R(t)]+\varepsilon(1-\delta_{\Omega\Omega'})\begin{pmatrix}J' & l & J\\ -\Omega' & 2 & -\Omega\end{pmatrix}\exp(\mathrm{i}\varpi^{\Delta\Omega=1}_{J'J}t)V_{l,2}[R(t)]\right\}, \quad (8)\end{aligned}$$

where $[R(t)]$ is the distance from the atom to the mass centre of the diatom, ϖ is the energy difference in the $J \to J'$ transition.

The unpolarized transition probability can be written as[32,34,35]

$$P_{JJ'} = \frac{1}{(2J+1)} \sum_{LL'} \left| \frac{1}{\mathrm{i}\hbar} \int_{-\infty}^{\infty} \left\langle J'\Omega'\varepsilon'^2 \Pi'_\Omega \Im\varsigma \right| V(t) \left| J\Omega\varepsilon^2 \Pi_\Omega \Im\varsigma \right\rangle \mathrm{d}t \right|^2 . \tag{9}$$

Introducing Eq.(8) into Eq.(9), one can obtain an explicit formula for the $J \to J'$ transition probability[19]

$$P_{JJ'} = P_{JJ'}^{\Delta\Omega=0} + P_{JJ'}^{\Delta\Omega=1} + 2\varepsilon \sum_l [(P_{JJ'}^{\Delta\Omega=0})_l]^{1/2} [(P_{JJ'}^{\Delta\Omega=1})_l]^{1/2}. \tag{10}$$

Equation (10) also can be written in the form given in Refs.[1], [7] and [8]

$$P_{JJ'} = P_{JJ'}^{\Delta\Omega=0} + P_{JJ'}^{\Delta\Omega=1} + 2\varepsilon (P_{JJ'}^{\Delta\Omega=0} P_{JJ'}^{\Delta\Omega=1})^{1/2} \cos\theta^D, \tag{11}$$

with the differential interference angle

$$\cos\theta^D = \frac{\sum_l [(P_{JJ'}^{\Delta\Omega=0})_l]^{1/2} [(P_{JJ'}^{\Delta\Omega=1})_l]^{1/2}}{(P_{JJ'}^{\Delta\Omega=0} P_{JJ'}^{\Delta\Omega=1})^{1/2}}. \tag{12}$$

The velocity-averaged differential interference angle can be obtained[9,10,17]

$$\cos\theta^D_{\mathrm{AV}} = \frac{\int \sum_l [(P_{JJ'}^{\Delta\Omega=0})_l]^{1/2} [(P_{JJ'}^{\Delta\Omega=1})_l]^{1/2} v^3 \exp\left(\frac{-\mu v^2}{2kT}\right) \mathrm{d}v}{\left(\int P_{JJ'}^{\Delta\Omega=0} v^3 \exp\left(\frac{-\mu v^2}{2kT}\right) \mathrm{d}v\right)^{1/2} \left(\int P_{JJ'}^{\Delta\Omega=1} v^3 \exp\left(\frac{-\mu v^2}{2kT}\right) \mathrm{d}v\right)^{1/2}}. \tag{13}$$

We consider that the differential interference angle may be closely related to the orbit angular momentum mentioned above. But the differential interference angles given in Eqs.(12) and (13) are correct descriptions of a molecule in a $^2\Pi$ electronic state only when the magnitude of the spin–orbit constant A is infinitely large compared to the product of the rotational constant B multiplied by the total angular momentum quantum number J. When $B \times J > A$, $^2\Pi$ electronic state will result in Hund's case(b) limit.[17] Now further theoretical study of the collision-induced Λ-related quantum interference in rotational energy transfer in an atom–diatom system and a dynamic model of atom-$^2\Pi$[case(b)] diatomic molecules system is under way.

3. Results and discussion

In a molecular beam experiment, the relative velocity of the gases is uniform and can be controlled, so the differential interference angle can be measured. The scattering angle is sensitive to the impact parameter and the potential energy surface. To simplify the discussion, we adopt the anisotropic Lennard-Jones interaction in the space frame ($l \le 2$)

$$\begin{aligned} V_{A'}(R,\theta,\phi) =& V_1(R) \sum_m [a_{1,0} {D^1_{m,0}}^*(\Omega) C^1_m(\theta,\phi)] \\ &+ V_2(R) \sum_m [a_{2,0} {D^2_{m,0}}^*(\Omega) C^2_m(\theta,\phi) \\ &+ a_{2,2} {D^2_{m,2}}^*(\Omega) C^2_m(\theta,\phi)] \end{aligned} \tag{14}$$

with

$$V_1(R) = 4d\left[(\sigma/R)^{12} - (\sigma/R)^7\right], \tag{15}$$

$$V_2(R) = 4d\left[(\sigma/R)^{12} - (\sigma/R)^6\right], \tag{16}$$

where the parameters d and σ represent the potential-well depth and the collision diameter, respectively; $a_{l,k}$ is the anisotropic parameters. For a $^2\Pi$ diatomic molecule, $\Lambda = \pm 1$ and $\Sigma = \pm 1/2$. If Λ and Σ are parallel to each other, $|\Omega| = 3/2$. If not, $|\Omega| = 1/2$. To simplify the discussion, we take $|\Omega| = 1/2$. For the experiments of NO($X^2\Pi$) with He, Ne and Ar, one can obtain the interference angle for $J' = J \pm 1$. For example, when $J' = J + 1$, the interference angle of Eq.(12) is[17]

$$\cos\theta^D = \frac{A}{B^{1/2} C^{1/2}}, \tag{17}$$

$$A = \left| \frac{\sigma^6}{b^{11}} F_6(x^{\Delta\Omega=0}) - \frac{1}{b^5} F_3(x^{\Delta\Omega=0}) \right| \times \left[\frac{\sigma^6}{b^{11}} F_6(x^{\Delta\Omega=1}) - \frac{1}{b^5} F_3(x^{\Delta\Omega=1}) \right], \tag{18}$$

$$B = \frac{(a_{10})^2 \sum_{L,L'} (2L'+1) \begin{pmatrix} L' & 1 & L \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} J & L & \Im \\ L' & J' & 1 \end{Bmatrix}^2 \begin{pmatrix} J' & 1 & J \\ -1/2 & 0 & 1/2 \end{pmatrix}^2}{(a_{20})^2 \sum_{L,L'} (2L'+1) \begin{pmatrix} L' & 2 & L \\ 0 & 0 & 0 \end{pmatrix}^2 \begin{Bmatrix} J & L & \Im \\ L' & J' & 2 \end{Bmatrix}^2 \begin{pmatrix} J' & 2 & J \\ -3/2 & 2 & -1/2 \end{pmatrix}^2}$$
$$\times \left| \frac{\sigma^6}{vb^{11}} F_6(x^{\Delta\Omega=0}) - \frac{1}{vb^5} F_{7/2}(x^{\Delta\Omega=0}) \right|^2 + \left| \frac{\sigma^6}{vb^{11}} F_6(x^{\Delta\Omega=1}) - \frac{1}{vb^5} F_3(x^{\Delta\Omega=0}) \right|^2, \tag{19}$$

$$C = \left[\frac{\sigma^6}{b^{11}} F_6(x^{\Delta\Omega=1}) - \frac{1}{b^5} F_3(x^{\Delta\Omega=1}) \right]^2. \tag{20}$$

From Eqs.(17)–(20), the differential interference angle of rotational energy transfer of NO($X^2\Pi$) in Hund's case (a) induced by collision with He, Ne and Ar atoms can be calculated quantitatively. (The needed parameters for the calculation are listed in Table 1)

Table 1. Parameters for the theoretical calculation of the integral interference angle $\theta_{\rm ST}^{\rm I}$.

Collision system	Reduced Mass/a.u.	σ/nm	$b_{\min}$/nm	$L = \mu v b/\hbar = \frac{\mu b}{\hbar}\sqrt{\frac{8kT}{\pi\mu}}$			B/cm^{-1}
				T=77	T=181	T=253	
NO–He	3.53	0.236	0.27	10	16	19	
NO–Ne	12.09	0.255	0.29	21	31	37	2.015[a]
NO–Ar	17.13	0.321	0.33	28	42	50	

[a] Rotation constant B from Ref.[21].

We have calculated the differential interference phase angles for NO($X^2\Pi$) in Hund's case (a) colliding with He, Ne and Ar atoms, from the initial rotational state J to the final rotational state $J' = J + 1$. The ratio of anisotropic parameters ($a_{1,0}/a_{2,0}$) used in our calculation is 0.1, because the ratio of $a_{1,0}/a_{2,0}$ for NO($X^2\Pi$) colliding with He, Ne and Ar atoms is $0.08 \le a_{1,0}/a_{2,0} \le 0.12$.[17,19] The greatest value of b is chosen to be 0.8 nm. When $b > 0.8$ nm, the interaction between atom and diatom almost disappears. The calculated values are plotted in Fig1.

1) In Fig.1, we can see that the variation of the differential interference angle with the impact parameter b is not monotonic. We give the interpretation of the interference angles variation as below: a). The probability of rotational energy transfer and interference will increase with the duration of collision, and the impact parameter just plays a key role in affecting the duration. b). The energy interval has a close connection with the impact parameter, and the larger impact parameter will bring an opposite effect to the interference. The two factors result in the variation of the differential interference angle in Fig.1.

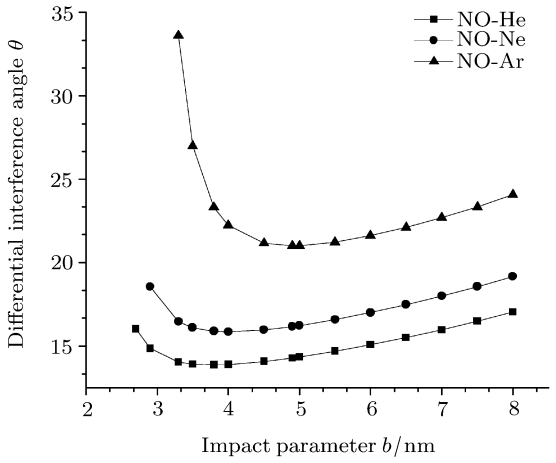


Fig.1. The variation of $\theta_{v=1000}^{D}$ with the impact parameter b for NO($X^2\Pi$) collision with He, Ne and Ar atoms at T=181 K and J=3/2.

2) The curve given in Fig.2 exhibits the tendency of the variation of interference angles, which is con-

sistent with the experimental results qualitatively.[1,2] Therefore, we give the interference angle change as below: 1) the collisional interaction increases with the increase of the rotational quantum number; 2) due to the collision perturbation, there will be different energy level shifts during the spin-orbit conserving transition and the spin-orbit changing transition; and 3) this will result in the decoupling of the spin-orbit mixed states. As a result of decoupling, the degree of mixing of corresponding wavefunctions will become much smaller than that of the isolated molecules and the interference effect will become weaker as well.

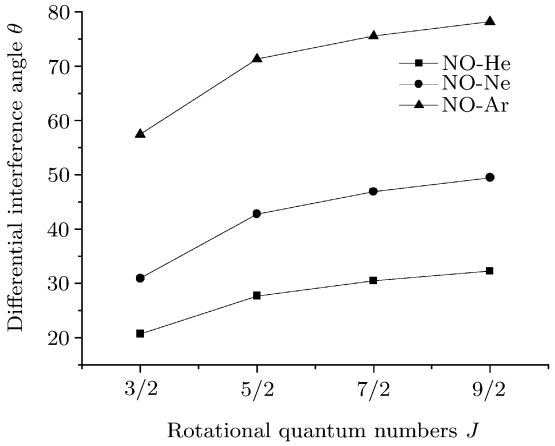


Fig.2. The variation of the $\theta^D_{\rm AV}$ with the rotational quantum number J at $b = b_{\rm min}$ and T=181 K.

3). With the increase of orbit angular momentum (i.e., with the increase of mass of partner, impact parameter, or experimental temperature), the interference angle decreases, because of $L = \mu v b/\hbar = (ub/\hbar)(8kT/\pi\nu)^{1/2}$ and $\mu = m_{\rm NO}m_{\rm partner}/(m_{\rm NO} + m_{\rm Partner})$. So the quantum interference effect of rotational energy transfer increases, as shown in Fig.3. We think that the orbit angular momentum and the relative velocity depend on the experimental temperature. The former influences the electrostatic interaction potential between the atom and diatom. The mixing degree of corresponding wavefunctions will become much bigger than that of the isolated molecules due to the increase of the temperature, and the interference effect will become stronger as well.

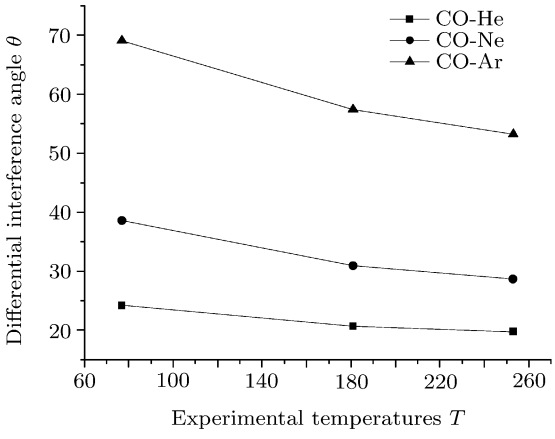


Fig.3. The variation of $\theta^D_{\rm AV}$ with the experimental temperature T at J=3/2 and $b = b_{\rm min}$.

4). We also obtain the variation of $\theta^D_{\rm AV}$ and $\theta^D_{v=921}$ with the impact parameter b, which is consistent with the experimental results qualitatively.[1,2] $\theta_{\rm AV}$ is the velocity-averaged differential interference angle and $\theta_{v=921}$ is the differential interference angle at the most probable velocity, 921 m/s.

As shown in Fig.4, the variation trend of $\theta_{\rm AV}$ is consistent with that of $\theta_{v=921}$. The greatest D-value between $\cos\theta_{\rm AV}$ and $\cos\theta_{v=921}$ is less than 0.017, namely, the contribution of the neighbourhood of most probable velocity to the energy transfer is the greatest and the effect of other places is very small.

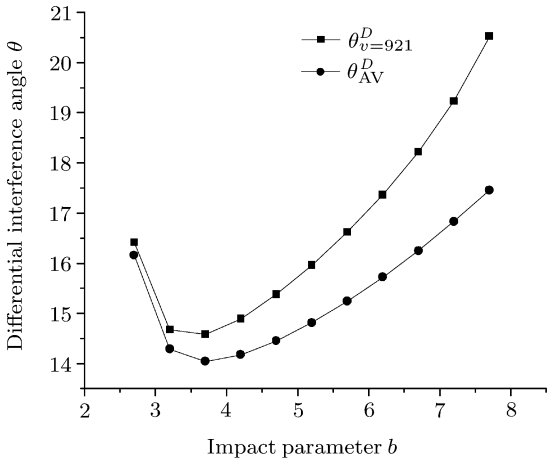


Fig.4. The variation of $\theta^D_{\rm AV}$ and $\theta^D_{v=921}$ with the impact parameter b for NO($X^2\Pi$) collision with He at J=3/2 and T=181 K.

4. Conclusions

Collisional quantum interference of the $^2\Pi$ electronic state, well described by Hund's case (a) on rotational energy transfer, which originates from the difference between the two Λ-related collision potential energy surfaces, was studied theoretically. Based on the time-dependent first-order Born approximation, and taking into account the anisotropic Lennard-Jones interaction potentials with 'straight-line' trajectory approximation, we have obtained the factors on which the interference angle depends, and the variation of the interference with them.

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