

# Collisional Quantum Interference on Rotational Energy Transfer : Relationship between Interference Angle and Relative Velocity<sup>\*</sup>

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**Abstract :** A dynamic model of collisional quantum interference (CQI) on rotational energy transfer in an atom-diatom system has been described by Sun *et al.* , based on the first order Born approximation of time dependent perturbation theory and long-range interaction potential. The experiment CO A  $\Pi$   $\Sigma^-$  collision with He in a static cell has been simulated successfully. To obtain directly the relationship between interference angle and relative velocity from experiment , an experiment is proposed by Sha , using molecular beam and velocity imaging technology. As a theoretical study of the relationship between interference angle and relative velocity , the interference angles are calculated with different relative velocities , and the changing tendency is obtained. It is revelatory for the molecular beam experiment to measure directly the interference angles by controlling the relative velocities.

**Key words :** Collisional quantum interference , Interference angle

**CLC number** O64      **Document code** : A

## 1 Introduction

Thanks to the ultrasensitive optical-optical double resonance multiphoton ionization technique ( the state-to-state cross sections have now become measurable to an accuracy of 10% )<sup>[1]</sup> , the evidence of collisional quantum interference ( CQI ) in intramolecular rotational energy transfer was obtained by Sha *et al.* in the CO A  $\Pi$  (  $v = 0$  )  $\Sigma^-$  (  $v = 1$  ) system in collision with He and other partners<sup>[2,3]</sup>. CQI was also observed by Chen *et al.* in Na<sub>2</sub> A  $\Sigma_u^+$  (  $v = 8$  )  $\Pi_{0u}$  (  $v = 14$  ) system in collision with Na ( 3s )<sup>[4]</sup>.

In the study of state-resolved collision-induced electronic transitions , three models have been proposed. Gilbert and Freed first proposed the 'gateway' model<sup>[5]</sup>

$$\sigma_{EJ, E'J} \approx C_{EE'}(J)^2 \sigma_{EJ, E'J} + C_{EE'}(J)^2 \sigma_{E'J, E'J} \quad (1)$$

where  $\sigma_{EJ, E'J}$  and  $\sigma_{E'J, E'J}$  are cross sections for pure collision-induced rotational transitions within the two electronic states ,  $C_{EE'}(J)^2$  and  $C_{EE'}(J)^2$  are the isolated-molecule  $EE'$  mixing coefficients induced by non-Born-Oppenheimer interactions. Alexander *et al.* pointed out that transition amplitudes between the basis state components of  $E$  and  $E'$  should first be summed and then squared to obtain the transition probabilities or the cross-sections rather than the reverse<sup>[6]</sup>. There should appear a cross term that represents the interference effect between the transition channels ,

$$\sigma_{JJ} = c_J^2 c_J^2 \sigma_{JJ}^S + d_J^2 d_J^2 \sigma_{JJ}^T +$$

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$$2c_j c_{j'} d_j d_{j'} (\sigma_{j'j}^S \sigma_{jj'}^T)^{1/2} \quad (2)$$

where  $c$  and  $d$  are the mixing coefficients,  $\sigma_{j'j}^S$  and  $\sigma_{jj'}^T$  are the energy transfer cross sections for pure singlet and triplet states, respectively. The first and second terms represent the contribution of singlet and triplet channels, respectively, and the last is the interference term. Based on the time-dependent first order Born approximation, Sha *et al.* proposed the third model which shows explicitly the interference effect by a cross term<sup>[23]</sup>,

$$\sigma_{j'j} = c_j^2 c_{j'}^2 \sigma_{j'j}^S + d_j^2 d_{j'}^2 \sigma_{jj'}^T + 2c_j c_{j'} d_j d_{j'} (\sigma_{j'j}^S \sigma_{jj'}^T)^{1/2} \cos \theta_{ST} \quad (3)$$

where  $\cos \theta_{ST}$  measures the degree of coherence, and  $\theta_{ST} \equiv |\theta_S - \theta_T|$ ,  $\theta_S$  and  $\theta_T$  represent the respective phase changes for the singlet and triplet transition channels.

The experiment CO A  $\Pi(v=0) \rightarrow \Sigma^-(v=1)$  system in collision with He and other partners were done in a static cell<sup>[23]</sup>, so the relative velocity between CO and partners are in Maxwell-Boltzmann distribution. If experiments can be conducted in molecular beams, the collisional quantum interference effect might be able to be observed more precisely<sup>[21]</sup>, because the velocity is uniform and can be controlled.

To control the interference angles by the uniform relative velocities, an experiment is proposed by Sha<sup>[71]</sup>, using molecular beam and velocity imaging technology. As a theoretical study of the relationship between interference angle and relative velocity, using Sun's model (the experiment CO A  $\Pi \rightarrow \Sigma^-$  collision with He in a static cell has been simulated successfully)<sup>[81]</sup>, the interference angles of experiment CO A  $\Pi \rightarrow \Sigma^-$  collision with He in condition of molecular beam are calculated, and the changing tendency of them is obtained.

## 2 Theory

The Born-Oppenheimer electronic Hamiltonian is written in the form,

$$H_e = H_A + H_B + V \quad (4)$$

where  $H_A$  and  $H_B$  are the electronic Hamiltonians of atom A and molecule B, and  $V$  represents the electrostatic interaction potentials. In this paper, only long-range interaction is considered, and because atom A

has no permanent multipole moments,  $V$  in Eq.(4) are limited to the induction potential and the dispersion potential<sup>[81]</sup>

$$V = V_{\text{ind}} + V_{\text{dis}} \\ = -B_1 R^{-6}(t) - B_2 R^{-6}(t) \times \\ \sum_{M_L} (-1)^{2-M_L} D_{M_L,0}^{2,0}(\Omega_2) C_{M_L}^2(\Omega_t) \quad (5)$$

$$\left\{ \begin{array}{l} B_1 = \frac{1}{3} \xi_{1,1}^0 R_{1,1}^{00}(\alpha_{XX} + \alpha_{YY} + \alpha_{ZZ})_A \times \\ \left[ \frac{1}{2}(\mu_X^2 + \mu_Y^2 + \mu_Z^2) + \frac{1}{4} \times \right. \\ \left. \frac{I_1 I_2}{I_1 + I_2} (\alpha_{XX} + \alpha_{YY} + \alpha_{ZZ}) \right]_B \\ B_2 = \frac{1}{3\sqrt{10}} \xi_{1,1}^0 R_{1,1}^{20}(\alpha_{XX} + \alpha_{YY} + \alpha_{ZZ})_A \times \\ \left[ \frac{1}{2}(\mu_X^2 + \mu_Y^2 - 2\mu_Z^2) + \frac{1}{4} \times \right. \\ \left. \frac{I_1 I_2}{I_1 + I_2} (\alpha_{XX} + \alpha_{YY} - 2\alpha_{ZZ}) \right]_B \end{array} \right. \quad (6)$$

where  $\xi$  is a purely algebraic coefficient<sup>[9]</sup>,  $\alpha$ ,  $\mu$  and  $I$  are polarizability, dipole moment and the first ionization potential respectively,  $D_{M,K}^L$  is the Wigner  $D$  rotation matrix, and  $C_M^L(\Omega)$  is a Racah harmonic function. The evolution of the interaction potential is<sup>[10]</sup>

$$V(t) = U^\dagger(t, \rho) V U(t, \rho) \quad (7)$$

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

$$U(t, \rho) = \exp\left(-\frac{iH_0 t}{\hbar}\right) \quad (8)$$

with

$$H_0 = \hbar\omega = hc \bar{B} J(J+1) \quad (9)$$

where  $\bar{B}$  is the rotation constant of molecule B,  $J$  is the rotation quantum number.

In order to simplify the notation, we consider collisions of molecule B with a structureless perturber (atom A) i.e.; we ignore the rotational and vibrational degrees of freedom of the perturber. The perturber are assumed to have electronic excitation energies which are much higher in energy than the molecule B, so electronic energy transfer process may be ignored. The unperturbed wave functions are

$$\begin{pmatrix} \varphi_j^S \\ \varphi_j^T \end{pmatrix} = \begin{pmatrix} |\nu^S \rangle |JKM^S\rangle \\ |\nu^T \rangle |JKM^T\rangle \end{pmatrix} \quad (10)$$

where  $|\nu^S\rangle$  and  $|JKM^S\rangle$  represent the vibration and rotation wave function respectively. The zeroth order unperturbed energies are defined as  $E(\varphi_j^S)$  and  $E$

( $\varphi_j^T$ ). If  $\nu_{ST}$  is the coupling between these zeroth order states, the perturbed states have energies<sup>[11]</sup>,

$$E_{\pm}(JKM) = \frac{1}{2}[E(\varphi_j^S) + E(\varphi_j^T)] \pm \frac{1}{2}\{[E(\varphi_j^S) - E(\varphi_j^T)]^2 + 4\nu_{ST}^2\}^{1/2} \quad (11)$$

The perturbed wave functions are

$$\begin{pmatrix} \psi_j^S \\ \psi_j^T \end{pmatrix} = \begin{pmatrix} \cos\phi_j & \sin\phi_j \\ -\sin\phi_j & \cos\phi_j \end{pmatrix} \begin{pmatrix} \varphi_j^S \\ \varphi_j^T \end{pmatrix} \quad (12)$$

Eq.(11) shows that the mutual perturbing states are repulsive each other. The energy level shifts  $\Delta_{\pm}$  is,

$$\Delta_{\pm} \equiv E_{\pm}(JKM) - E(\varphi_j) \quad (13)$$

where  $\Delta_+$  denotes an upward shift and  $\Delta_-$  a downward shift. The argument  $\phi$ , characterizing the mixing effects, is given by,

$$\phi = \arctan\left(\frac{\nu_{ST}}{E(\psi_j^S) - E(\psi_j^T)}\right) \quad (14)$$

In the later derivation, according to Eq.(11), we set that the mixing coefficients  $c_j \equiv \cos\phi_j$  and  $d_j \equiv \sin\phi_j$ , or  $c_j \equiv -\sin\phi_j$  and  $d_j \equiv \cos\phi_j$  depending on the perturbed state is a singlet or a triplet state. If both the initial state  $|i\rangle$  and final state  $|f\rangle$  of a collision-induced transition are singlet-triplet mixed states, then

$$|i\rangle = c_j |\nu^S\rangle |JKM^S\rangle + d_j |\nu^T\rangle |JKM^T\rangle \quad (15)$$

$$|f\rangle = c_j |\nu'^S\rangle |J'K'M'^S\rangle + d_j |\nu'^T\rangle |J'K'M'^T\rangle \quad (16)$$

According to the first-Born approximation of time dependent perturbation theory, the amplitude for a transition between  $|i\rangle$  and  $|f\rangle$  is,

$$\begin{aligned} \int |f\rangle V(t) |i\rangle dt &= -c_j c_j B_2^S \times \\ &\sum_{M_L} (-1)^{J-M_L} \langle J'K'M'^S | D_{M_L,0}^{2J} | JK M^S \rangle \times \\ &\int_{-\infty}^{\infty} \exp(i\omega_{jT}^S t) R^{-\zeta}(t) C_{M_L}^2(\Omega_t) dt - d_j d_j B_2^T \times \\ &\sum_{M_L} (-1)^{J-M_L} \langle J'K'M'^T | D_{M_L,0}^{2J} | JK M^T \rangle \times \\ &\int_{-\infty}^{\infty} \exp(i\omega_{jT}^T t) R^{-\zeta}(t) C_{M_L}^2(\Omega_t) dt \quad (17) \end{aligned}$$

where only electrostatic interaction is involved with no magnetic coupling present, i.e., a transition between  $\Lambda \Pi$  and  $e \Sigma^-$  state is prohibited<sup>[2,7]</sup>. In Eq.(17), the vibration factor  $\langle \nu' | \nu \rangle = 1$  has been omitted, because only the rotational energy transfer is considered

( $\langle \nu'^S | \nu^S \rangle = \langle \nu'^T | \nu^T \rangle$ ). The rotational matrix element in Eq.(17) is,

$$\langle J'K'M'^S | D_{M_L,0}^{2J} | JK M^S \rangle = [(2J+1) \times (2J'+1)]^{1/2} \begin{pmatrix} J & 2 & J \\ M' & -M_L & M \end{pmatrix} \begin{pmatrix} J & 2 & J \\ K' & 0 & K \end{pmatrix} \quad (18)$$

The integral in Eq.(17)

$$I_{M_L}^L = \int_{-\infty}^{\infty} \exp(i\omega_{jT} t) R^{-\zeta}(t) C_{M_L}^L(\Omega_t) dt \quad (19)$$

has been done by Gray and Kranendonk in a "straight-line" trajectory approximation  $R(t) = (\nu^2 t^2 + b^2)^{1/2}$ <sup>[12]</sup>, by introducing the dimensionless variables,

$$x = \frac{\omega b}{\nu}, \quad z = \frac{\nu t}{b} \quad (20)$$

where  $b$  and  $\nu$  are the impact parameter and the relative velocity in the center of mass coordinate system respectively. The result of the integral is

$$I_{M_L}^L = b^{-5} \nu^{-1} J_{M_L}^L(x) \quad (21)$$

$$J_{M_L}^L = i^{L-M_L} A_{M_L}^L(x) \quad (22)$$

When  $L=2$  and  $M_L=0, 1, 2$ ,  $A_{M_L}^L(x)$  are,

$$\begin{aligned} A_0^2(x) &= \frac{3}{2} F_4(x) - F_3(x), \\ A_1^2(x) &= \left(\frac{3}{2}\right)^{1/2} G_4(x), \\ A_2^2(x) &= \left(\frac{3}{8}\right)^{1/2} F_4(x) \quad (23) \end{aligned}$$

$$\left\{ \begin{aligned} F_n(x) &= \frac{\pi}{(n-1)! 2^{2n-2}} e^{-x} \times \\ &\sum_{k=0}^{n-1} \frac{(2n-2-k)!}{k!(n-1-k)!} (2x)^k \\ G_n(x) &= \frac{\pi}{(n-1)! 2^{2n-3}} x e^{-x} \times \\ &\sum_{k=0}^{n-2} \frac{(2n-4-k)!}{k!(n-2-k)!} (2x)^k \end{aligned} \right. \quad (24)$$

Introducing Eq.(18) & (21) into Eq.(17), we can obtain,

$$\begin{aligned} \int |f\rangle V(t) |i\rangle dt &= -c_j c_j B_2^S \times \\ &\sum_{M_L} (-1)^{J-M_L} [(2J+1) \times (2J'+1)]^{1/2} \times \\ &\begin{pmatrix} J & 2 & J \\ M' & -M_L & M \end{pmatrix} \begin{pmatrix} J & 2 & J \\ K' & 0 & K \end{pmatrix} b^{-5} \nu^{-1} J_{M_L}^2(x^S) - \\ &d_j d_j B_2^T \sum_{M_L} (-1)^{J-M_L} [(2J+1) \times (2J'+1)]^{1/2} \times \\ &\begin{pmatrix} J & 2 & J \\ M' & -M_L & M \end{pmatrix} \begin{pmatrix} J & 2 & J \\ K' & 0 & K \end{pmatrix} b^{-5} \nu^{-1} J_{M_L}^2(x^T) \quad (25) \end{aligned}$$

The unpolarized state-to-state transition probability can be obtained by summing over initial and final molecular magnetic quantum numbers and by average over the initial ones<sup>[11]</sup>,

$$P_{JJ'} = \frac{1}{2J+1} \sum_{M'M} \left| \frac{1}{i\hbar} \int f | V(t) | i dt \right|^2 \quad (26)$$

Introducing Eq.(25) into Eq.(26) and considering the orthogonal relations involving the 3j symbols,

$$\sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{\delta_{j_3 j_3'} \delta_{m_3 m_3'}}{2j_3 + 1} \quad (27)$$

and Clebsch-Gordan coefficients,

$$\sum_{m_1 m_2} j_1 m_1 j_2 m_2 \begin{vmatrix} j_3 m_3 & j_1 m_1 j_2 m_2 \\ j_3' m_3' \end{vmatrix} = \delta_{j_3 j_3'} \delta_{m_3 m_3'} \quad (28)$$

and taking into account the relationship of coherent controlling<sup>[13]</sup>,

$$\int_0^{2\pi} d\varphi \exp[i\alpha(M^S - M^T)\varphi] = 2\pi \delta_{M^S M^T} \quad (29)$$

we obtain an explicit formula for the  $J \rightarrow J'$  transition probability<sup>[8]</sup>:

$$P_{JJ'} = c \hat{q} \hat{P}_{JJ'}^S + d \hat{q} \hat{P}_{JJ'}^T + 2c_{J'J} d_J d_{J'} \sum_{M_L} [ (P_{JJ'}^S)_{M_L} (P_{JJ'}^T)_{M_L} ]^{1/2} \cos\theta_{ST} = \frac{\int \sum_{M_L} \frac{1}{b^9} | J \mathcal{E}_{M_L^X T} \rangle | J \mathcal{E}_{M_L^X S} \rangle | db}{\left( \int \frac{1}{b^9} \sum_{M_L} | J \mathcal{E}_{M_L^X S} \rangle |^2 db \right)^{1/2} \left( \int \frac{1}{b^9} \sum_{M_L} | J \mathcal{E}_{M_L^X T} \rangle |^2 db \right)^{1/2}} \quad (30)$$

### 3 Result and discussion

The proposal of experiments in a molecular beam has been discussed by Sha *et al.*<sup>[7]</sup>. In a molecular beam, the velocity of the gases is uniform and can be controlled, so the interference angle can be measured directly from experiment according to different velocity, and also can be simulated theoretically by Eq.

$$\cos\theta_{ST} = \frac{\int \frac{1}{b^9} | J \mathcal{E}_{M_L^X T} \rangle | J \mathcal{E}_{M_L^X S} \rangle | db}{\left( \int \frac{1}{b^9} \sum_{M_L=0, \pm 2} | J \mathcal{E}_{M_L^X S} \rangle |^2 db \right)^{1/2} \left( \int \frac{1}{b^9} | J \mathcal{E}_{M_L^X T} \rangle |^2 db \right)^{1/2}} \quad (35)$$

The parameters needed for the calculation are listed in Table 1. The calculated values for the initial rotational quantum number  $J = 9$  and the final quantum number,  $J' = 8$ ,  $J' = 10$  are presented in Fig. 1. From Fig. 1, we can see the interference angles increase with the increase of the relative velocity. This

$$P_{JJ'}^H = \frac{B_2^H}{\hbar^2 v^2 b^{10}} \frac{2J'+1}{2L+1} \begin{pmatrix} J' & 2 & J \\ K' & 0 & K \end{pmatrix}^2 \sum_{M_L} | J_{M_L}^2(x_H) |^2 \quad (31)$$

where  $L = 2$ . In above Eq., H stands for S or T. The energy transfer cross section can be expressed as<sup>[14]</sup>,

$$\sigma_{JJ'} = 2\pi \int_0^\infty P_{JJ'}(b) b db \quad (32)$$

By introducing Eq.(30) into Eq.(32), the integral cross-section Eq.(3) can be obtained,

$$\sigma_{JJ'} = c \hat{q} \hat{q}_{JJ'}^S + d \hat{q} \hat{q}_{JJ'}^T + 2c_{J'J} d_J d_{J'} ( \sigma_{JJ'}^S \sigma_{JJ'}^T )^{1/2} \cos\theta_{ST}$$

with cosine of the interference angle,

$$\cos\theta_{ST} = \frac{\int \sum_{M_L} [ (P_{JJ'}^S)_{M_L} (P_{JJ'}^T)_{M_L} ]^{1/2} b db}{\left( \int (P_{JJ'}^S(b) b db \right)^{1/2} \left( \int (P_{JJ'}^T(b) b db \right)^{1/2}} \quad (33)$$

By introducing Eq.(32) into Eq.(33) and reducing  $B_2^S$  and  $B_2^T$ , which are independent of  $v$  and  $b$  as can be seen from Eq.(6), an explicit formula for  $\cos\theta_{ST}$  is obtained,

$$\cos\theta_{ST} = \frac{\int \sum_{M_L} \frac{1}{b^9} | J \mathcal{E}_{M_L^X T} \rangle | J \mathcal{E}_{M_L^X S} \rangle | db}{\left( \int \frac{1}{b^9} \sum_{M_L} | J \mathcal{E}_{M_L^X S} \rangle |^2 db \right)^{1/2} \left( \int \frac{1}{b^9} \sum_{M_L} | J \mathcal{E}_{M_L^X T} \rangle |^2 db \right)^{1/2}} \quad (34)$$

(34). In calculation of interference angle for the experiment CO A  $\Pi_e \Sigma^-$  collision with He, the first summation in the denominator is for  $\Pi$  channel, so  $M_L = 0$  and  $M_L = \pm 2$  (the  $C_{2v}$  symmetry of the  $\Pi$  electron change distribution can be reflected by the symmetry of the potential function<sup>[15,16]</sup>; the second summation in the denominator is for  $\Sigma^-$  channel,  $M_L = 0$  only. So the interference angle can be written as

tendency is consistent with the experimental results in the static cell<sup>[2,3]</sup> and the calculated values<sup>[8]</sup>: when the experimental temperatures increase, the relative velocity increases and the interference angles also increase. This

tendency can be explained : with the increase of the velocities , the time duration of collision is smaller , the probability of rotational energy transfer also decreases , so the interference also decreases , i. e. , the interference angles increase.

Table 1 Parameters for the theoretical calculation of the interference angle

Collision system	Reduced mass /a. m. u.	Rotational constant/cm <sup>-1</sup> [17]		$b_{\min}/\bar{v}^*$
		CO A II	CO e $\Sigma^-$	
CO-He	3.5	1.6105	1.2836	2.9

\*  $b_{\min}$  is the minimum value of impact parameter , from Ref. [ 18 ]

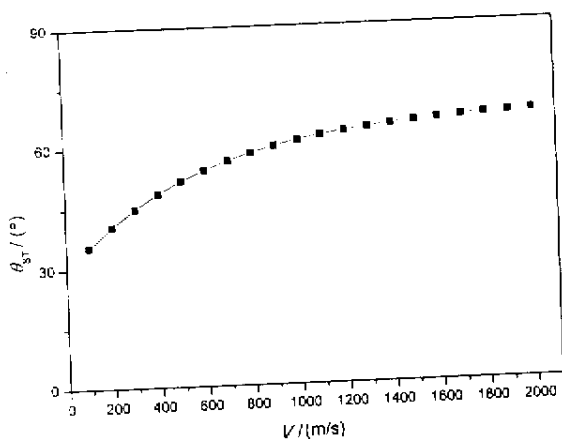


Fig.1 Relationship between the interference angles and the relative velocities

The last term of Eq.(3) is the interference term and  $\cos\theta_{ST}$  measures the degree of coherence between two channels. CQI is different from other quantum interference , such as electronic diffraction. It is interesting to compare CQI with electronic diffraction. CQI and electronic diffraction both belong to an interference between de Brogie waves( matter waves ), but the interference of electronic diffraction is in a space of momentum , while CQI is in a space of angular momentum ; the translational motion of electronic is a travelling wave , while the rotational motion of molecule is a stationary wave , and the length of wave

$$\text{is } \lambda = \frac{2\pi r}{\sqrt{J(J+1)}} \quad [3]$$

The nature of the experiment proposed by Sha , using molecular beam and velocity imaging technology , is one of controlling process of chemical reaction :

controlling the interference angle by the relative velocity with a molecular beam. But CQI is different from other chemical reaction controlled by laser , such as Bose-Einstein condense , coherent control approach for control dynamical processes<sup>[19-21]</sup>. CQI is a radiationless transition process , while the others results from the interaction of light with an atom or a molecule<sup>[4]</sup>.

In this paper , several approximations are used :

( 1 ) The translational motion is treated classically , whereas vibrational and rotational motions are handled quantum mechanically. Treating translational motion classically is a good approximation if the wave packet for the relative translational motion does not broaden appreciably during the collision.

( 2 ) In integrating over the impact parameter , the straight-line trajectory approximation proposed by Gray and van Kranendonk<sup>[12]</sup> is used. This approximation requires that the energy transferred to the internal degrees of freedom is much less than the energy of relative translational motion.

( 3 ) The probability of rotational energy transfer is derived using the first order Born approximation of time dependent perturbation theory. This is a good approximation if ( i ) the kinetic energy of the relative motion is much greater than the potential energy , ( ii ) the probability of rotational energy transfer is small.

The validity of these approximations has been discussed detailedly<sup>[7]</sup>.

## 4 Summary

Using Sun's dynamic model of CQI , the relationship between interference angle and relative velocity is obtained theoretically. It is revelatory for the molecular beam experiment to measure directly the relationship between interference angle and relative velocity , using molecular beam and velocity imaging technology.

**Acknowledgements :** This work was supported by NNSFC( 29973045 ) and NKBRSF.

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## 转动传能中的量子干涉：干涉角和相对速度的关系\*

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摘要：考虑一级含时波恩近似和长程相互作用势，Sun 提出了转动传能中的量子干涉模型。在静态池中 CO  $A^1\Pi e \Sigma^-$  和 He 碰撞的实验已经成功模拟。为了从实验中直接获得碰撞速度和干涉角的关系，Sha 提出了利用分子束和离子速度成像技术的实验。作为理论研究干涉角和碰撞速度的关系，计算了不同速度下的干涉角，同时获得了变化的趋势。对在分子束条件下(通过控制碰撞速度来控制干涉角)实验具有指导意义。

关键词：碰撞量子干涉；干涉角

中图分类号：O64 文献标识码：A

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