Excitation Functions in Low-Energy $\text{He}^+ - \text{He}$ Collisions

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In order to study the relations between the profile of excitation function and excitation mechanism, the equations of rotational coupling and radial coupling have been solved with various forms of transition moment and potential energy curve in the two-level model. The excitation functions populated by the rotational coupling through potential curve crossings at small internuclear distance increase gradually with increasing of ion energy and hardly show clear threshold. On the other hand, the excitation functions of the radial coupling increase rapidly near threshold energy and take their maximum values at low colliding energy compared with those of rotational coupling. These characteristics originating from the excitation mechanisms have been recognized on the profiles of the observed emission cross sections.

1. Introduction

On the studies of emissions generated by heavy particle collisions, such as beam-gas and beam-solid collisions and some processes in hot plasmas, we refer the excitation functions of relevant processes, and find various profiles of excitation functions. Are there any correlations between the profiles of excitation functions and the excitation mechanisms?

Investigations of emission cross section of $\text{He}^+ - \text{He}$ collisions which is, from experimental point of view, the simplest colliding system of heavy particles except $\text{H}^+ - \text{He}$ are very useful to analyse the excitation mechanism in heavy particle collisions. In low-energy colli-

sions of $10\text{--}10^4\text{ eV}$, the excitations occur as transitions between the quasi-molecular states those are composed of the colliding particles at small internuclear distance and the transitions arise preferentially near the crossing points of electronic potential energy curves of quasi-molecules. Since highly excited levels of the molecules interact with many nearby levels through successive crossings of potential curves, the excitation cross sections of the levels show complicated structures on energy dependence. On the other hand, the potential curves of lower excited levels cross only few low-lying potential curves and distinguishable contribution of each crossing possibly appears on the cross sections. In facts, the observed

energy dependences of emission cross sections from low-lying excited levels in $\text{He}^+ - \text{He}$ collisions are comparatively simple¹⁻³⁾ and the main structures of them are classified into two types¹⁾; the emission cross section increases gradually without clear threshold, as ion energy increases, and does not reach its maximum at ion energy less than several hundreds eV (*type A*). In another type, the emission cross section increases abruptly near threshold energy and takes its maximum at few hundreds eV and slowly decreases (*type B*).

The purpose of the present paper is to make clear the relationships between the behaviors of the observed emission cross sections and the excitation mechanisms. We have performed numerical calculations of coupled equations of two type coupling schemes, the rotational coupling and the radial coupling, in the two-level model for the excitation of He I and He II levels. Then, we have shown that the calculated excitation functions well reproduce, with varying parameters included in the coupled equations, the profiles of the observed emission cross sections and that the characteristic behaviors of the cross sections excited by the rotational and the radial couplings agree with those of the observed cross sections of *type A* and *type B*, respectively.

Of course, absolute values of the cross sections obtained by this simple calculations are different from those by the close-coupling calculations,⁴⁻⁶⁾ but the present method is useful to make clear the role of atomic parameters, such as potential energy curve and transition moment, in the excitation processes.

2. The Coupled Equations in the Two-Level Model and the Correlation Diagram

In the molecular approach to ion-atom collision problems at low impact-energy, dynamic couplings of two types, rotational coupling and radial coupling, give rise to the transitions among the orbitals of the quasi-molecular states.⁷⁾ The transition moment of the rotational coupling is the matrix element of the component of the electronic angular momentum operator, in the body-fixed frame, which is perpendicular to the plane of the collision trajectory. This operator $L_{\perp}$ is also given as

$L_{\perp} = (L_+ - L_-)/2i$, where L_+ and L_- are raising and lowering operators for the angular momentum component along the internuclear axis and, hence, the selection rule for this type transition is $\Delta l = \pm 1$, such as Σ to Π and Π to Δ . The transition moment of the radial coupling is that of the derivative of internuclear distance $\partial/\partial R$. Since $\partial\Psi_i/\partial R$ has the same symmetry as Ψ_i , the selection rule for the radial coupling is $\Delta l = 0$, such as Σ to Σ and Π to Π . It is well known that transitions between states g to g or states u to u are allowed and transition from g to u states or from u to g states are forbidden for both of the radial and rotational coupling in symmetric collisions.

The coupled equations are described as follows. If $C_1(t)$ and $C_2(t)$ are the amplitudes of the initial and final components in the total wave function of the two-level model at time t , then in a collision with relative velocity v at an impact parameter ρ , the equations governing C_1 and C_2 for the rotational coupling are⁸⁾

$$\begin{aligned}\dot{C}_1 &= C_2 \frac{v\rho}{R^2} f_{\text{rot}}(R) \exp\left\{-\frac{i}{\hbar} \int_0^t (\epsilon_2 - \epsilon_1) d\tau\right\} \\ \dot{C}_2 &= -C_1 \frac{v\rho}{R^2} f_{\text{rot}}(R) \exp\left\{\frac{i}{\hbar} \int_0^t (\epsilon_2 - \epsilon_1) d\tau\right\},\end{aligned}\quad (1)$$

where R is internuclear distance and $f_{\text{rot}}(R) = \langle \Psi_1 | (i/\hbar) L_{\perp} | \Psi_2 \rangle$ is the matrix element above mentioned and ϵ_1 and ϵ_2 are the energies of the initial and the final molecular states, respectively. Equations for the radial coupling are

$$\begin{aligned}\dot{C}_1 &= C_2 v_R f_{\text{rad}}(R) \exp\left\{-\frac{i}{\hbar} \int_0^t (\epsilon_2 - \epsilon_1) d\tau\right\} \\ \dot{C}_2 &= -C_1 v_R f_{\text{rad}}(R) \left\{ \exp\left\{\frac{i}{\hbar} \int_0^t (\epsilon_2 - \epsilon_1) d\tau\right\} \right\},\end{aligned}\quad (2)$$

where $f_{\text{rad}}(R)$ is the matrix element $\langle \Psi_1 | \partial/\partial R | \Psi_2 \rangle$ and v_R is the velocity to the direction along the molecular axis.

The particles are assumed to move along the classical trajectory determined by the potential energy of the incoming channel, as described in equation 3.

$$\frac{dR}{dt} = \left\{ \frac{2E}{\mu} \left(1 - \frac{\rho^2}{R^2} - \frac{\epsilon_1(R)}{E} \right) \right\}^{1/2}, \quad (3)$$

here E is incident energy and μ is reduced mass. The coupled equations 1 and 2 are solved subject to the initial conditions $|C_1(-\infty)|=1$, $|C_2(-\infty)|=0$. The probability of the excitation during the collision is then given by $P(\rho)=|C_2(+\infty)|^2$, and the excitation cross section $\sigma(v)$ is

$$\sigma(v)=2\pi\int_0^\infty P(\rho)\rho d\rho. \quad (4)$$

If the quantities of $f(R)$'s, ϵ_1 and ϵ_2 are given, the equations 1 and 2 can be integrated numerically along an internuclear trajectory.

The diabatic correlation diagram of figure 1, which indicates the correlations between electronic configurations of the separated and united atom limits, brings about the general understanding of the excitation mechanisms of $\text{He}^+ - \text{He}$ collisions.⁹⁾ The incoming channel $1s\sigma_g\ 2p\sigma_u\ ^2\Sigma_{g^0}$ and the outgoing channel of $1s\sigma_g\ 2p\sigma_u\ 2p\pi_u\ ^2\Pi_{g1}$ dissociating to $\text{HeI}\ 2^1P$ at the separated atom limit and $1s\sigma_g\ 2p\sigma_u\ 2p\pi_u$

Fig. 1 Schematic correlation diagram of $\text{He}^+ - \text{He}$ system. The g -states relevant to the present studies are shown. The incident channel of $1s\sigma_g^2 2p\sigma_u \ ^2\Sigma_{u0}$ does not interact directly with the u -states dissociating to the excited levels interested.

${}^2\Pi_{g2}$ dissociating to $\text{HeI } 2^2P$ tend to the same united atom limit of $\text{BeII } (1s2p^2 \ ^2D)$. Consequently the potential curve crossings happen at small R and mechanism of excitation is the rotational coupling. The outgoing channels of $1s\sigma_g \ ^22s\sigma_g \ ^2\Sigma_{g1}$ dissociating into $\text{HeI } 2^3S$, $1s\sigma_g \ ^33s\sigma_g \ ^2\Sigma_{g2}$ dissociating into $\text{HeI } 3^3S$ and $1s\sigma_g \ ^55g\sigma_g \ ^2\Sigma_{g3}$ dissociating into $\text{HeI } 3^3D$, on the other hand, tend to other BeII levels and the potential curve crossings arise at comparatively large R . We have shown the radial coupling is important for excitation in this type crossings of low-energy collisions, though both of the rotational and radial coupling are possible.¹⁾ In order to investigate the origins of the characteristic energy dependences of the observed emission cross sections, we have examined the behaviors of the excitation functions resulting from above two types of

Fig. 2 Potential energy curves of quasi-molecular states. $V_0 = \{ (4/R) + 2.4 \} \exp(-1.33R)$,¹⁰⁾ this curve corresponds to $^2\Sigma_{g0}$ state in Fig. 1. $V_1 = V_0$ if $R \leq 1.2$ and $0.858 \exp(-0.6751R) + 0.7803$ if $1.2 < R$, $^2\Pi_{g1}$. $V_2 = V_0$ if $R \leq 0.6565$ and $10.0 \exp(-2.422R) + 1.5$ if $0.6565 < R$, $^2\Pi_{g2}$. $V_{2'} = V_0 + 0.375(8R - R^2)^{1/2}$ if $R \leq 4.0$ and $V_0 + 1.5$ if $4.0 < R$. $V_3 = \{ (4/R) - 3.2284 \} \exp(-2.03R) + 0.7284 + 0.18 \exp\{-\alpha(R - 1.7)^2\}$, $\alpha = 6.5$ if $R < 1.7$ and 0.325 if $1.7 < R$,¹³⁾ $^2\Sigma_{g1}$. $V_4 = V_0 - 1.474(R - 1.4)$. $V_5 = V_0 - 1.048(R - 1.4)^2$, $V_6 = V_0 - 0.5317(R - 1.4)^4$ if $R \leq 1.4$ and $V_4 = V_5 = V_6 = V_3$ if $1.4 < R$.

excitation processes.

3. Rotational Coupling

We considered excitations from $^2\Sigma_{g0}$ state only, because the direct excitation from the incoming channel is important in these types of collisions (see caption of figure 1). The lowest-energy of Σ_g symmetry calculated by Olson¹⁰⁾ was adopted as the energy ε_1 of the initial state $^2\Sigma_{g0}$ (curve V_0 in figure 2) in both calculations of rotational excitation and radial excitation. There are still more two undetermined parameters, $f_{\text{rot}}(R)$ and ε_2 , in the coupled equations.

3.1 Transition moments $f_{\text{rot}}(R)$

First, we have examined the dependence of excitation function of He I 2^1P on the form of transition moment $f_{\text{rot}}(R)$. Rather simple potential curve V_1 in figure 2 was assumed as the potential energy of the outgoing channel ε_2 . Trial forms of $f(R)$ are shown in figure 3. The curve f_b is scaled from the result of Bates and Sprevak¹¹⁾ who calculated the coupling element using approximate H_2^+ wave functions. The scaling is achieved by put $f_{He} = f(R_H/Z_{He})$ where R_H is the internuclear separation in the H_2^+ system and $Z_{He}=2$. Other curves in figure 3 are deformed from the curve f_b ; curve f_a

Fig. 3 Transition moments of the rotational coupling. $f_a=1.0$ if $R \leq 1.2$, $-0.417R+1.5$ if $1.2 < R \leq 3.5$ and $-6.25 \times 10^{-3}R+6.25 \times 10^{-2}$ if $3.5 < R$. f_b : scaled from $f(R)$ for H_2^+ system (see text).¹¹⁾ $f_c = -0.48R+1.0$ if $R \leq 2.0$ and $-5.08 \times 10^{-3}R+5.08 \times 10^{-2}$ if $2.0 < R$. $f_d = 0.833R$ if $R \leq 1.2$, $-5R+7.0$ if $1.2 < R \leq 1.4$ and 0 if $1.4 < R$.

Fig. 4 Excitation functions of He I 2^1P by rotational coupling in various forms of $f(R)$ and the observed emission cross section of He I $\lambda 584\text{\AA}$ (1^1S-2^1P) line. The curve a to d were derived from f_a to f_d in Fig. 3, respectively. Potential curves of V_0 and V_1 in Fig. 2 were used as ε_1 and ε_2 .

takes considerable value at large R compared with curve f_b and curve f_d takes finite value only near the crossing radius. The cross sections derived from these $f(R)$ and the fixed ε_2 of V_1 are shown in figure 4. In spite of considerable differences among $f(R)$'s, the cross sections show similar energy dependence. This means σ is relatively insensitive to the detailed form of the coupling element $f(R)$ and it agrees with the conclusion obtained by Briggs and Macek.¹²⁾ Then, we have used curve f_b for $f(R)$ in every coupled equations hereafter, unless otherwise specified.

Figure 5 shows the excitation probability as

Fig. 5 Excitation probabilities as function of impact parameter at various colliding energies for curve b in Fig. 4.

Fig. 6 Energy differences between the outgoing channel to $\text{HeII } 2^2P$ and the incoming channel V_0 , assumed in the calculation of rotational coupling. a : $V_2 - V_0$ in Fig. 2. $b = 0.698R^2$ if $R \leq 1.0$ and $V_2 - V_0$ in Fig. 2 if $1.0 < R$. $c = (b + d)/2$. d : $V_{2'} - V_0$ in Fig. 2.

function of impact parameter ρ for several impact energies, for examples.

3.2 Potential energies of the outgoing channel ϵ_2

Next, the influence of variation of the form of ϵ_2 exerted on the profile of the excitation function of $\text{HeII } 2^2P$ have been examined. Four kinds of potential energies for the $1s\sigma_g 2p\sigma_u 2p\pi_u {}^2\Pi_{g2}$ state were assumed as ϵ_2 and two of them are shown in figure 2 as curve V_2 and $V_{2'}$. The energy differences $\epsilon_2 - \epsilon_1$ of curve a to d in figure 6 indicate various approaches of ϵ_2 to ϵ_1 ; curve a derived from V_2 in figure 2 indicates that ϵ_2 degenerates with ϵ_1 at finite R and both energies take the same value at R less than 0.7 au. On curve b , ϵ_2 approaches rapidly to ϵ_1 , but does not degenerate with ϵ_1 except $R=0$. On curve d , which corresponds to potential curve $V_{2'}$ in figure 2, considerable amount of difference holds between ϵ_2 and ϵ_1 through whole internuclear distance and the curve c indicates the intermediate case between curve b and d .

Figure 7 indicates the cross sections calculated for above ϵ_2 's and the fixed $f(R)$ of curve f_b in figure 3. It shows that, in the measured range of ion energy, little variation of the potential energy curve results in very remarkable change on the cross section in comparison with the case of the variation of $f(R)$.

From the profiles of the excitation functions

Fig. 7 Excitation functions of $\text{HeII } 2^2P$ by rotational coupling in various forms of ϵ_2 and the emission cross section of $\text{HeII } \lambda 304\text{\AA}$ ($1^2S - 2^2P$) line. The curve a to d correspond to curve a to d in Fig. 6, respectively. $f_{\text{rot}}(R)$: f_b in Fig. 3.

in figure 4 and 7, we find the characteristics of the rotational excitation; the cross section increases gradually, as ion energy increases, without clear threshold, and it does not take its maximum in energy range less than several hundreds eV. The observed emission cross sections of $\text{HeI } \lambda 584\text{\AA}$ line ($1^1S - 2^1P$) and $\text{HeII } \lambda 304\text{\AA}$ line ($1^2S - 2^2P$) are shown in figure 4 and 7, respectively.¹⁾ They are normalized at the maximum values of the resembling excitation functions. The characteristics of the rotational excitation quite agree with the *type A* profile of the observed emission cross sections mentioned in section 1, which are also recognized on the cross section of $\lambda 584\text{\AA}$ and $\lambda 304\text{\AA}$ lines. The small structures on $\lambda 584\text{\AA}$ line cross section at low energy side seem to come from secondary excitation processes.¹⁾

Since profiles of the excitation functions are insensitive to the form of $f_{\text{rot}}(R)$, the profiles are mainly determined with the form of another parameter ϵ_2 . Conversely, we can determine the form of ϵ_2 by fitting the calculated excitation function to the observed cross section. The fitted excitation functions and the obtained potential energy curves ϵ_2 in this manner are shown in ref. 1.

4. Radial Coupling

The influence of form of $f_{\text{rad}}(R)$ and ε_2 on the profiles of excitation functions have been examined in the same manner as the preceding section.

4.1 Transition moments $f_{\text{rad}}(R)$

We used curve V_3 in figure 2 for the energy ε_2 , which is energy of the first excited level of $^2\Sigma_{g1}$ based on fits to energy-loss data for the excitation process $\text{He}^+ + \text{He} \rightarrow \text{He}^+ + \text{He}^*(2^3S)$.¹³⁾ As V_3 is a diabatic curve, we assumed a kind of pseudo-crossing between V_0 and V_3 , that is, ε_1 is V_0 in $R \geq R_0$ and V_3 in $R < R_0$, and ε_2 is V_3 in $R \geq R_0$ and V_0 in $R < R_0$ in our adiabatic calculations, where R_0 is the internuclear distance of the crossing point.

The parameter $f(R)$ was introduced from the theoretical results by other authors. The curve f_a and f_b in figure 8 correspond to the radial coupling terms of $\langle R\Gamma_1 | \frac{d}{dR} | R\Gamma_2 \rangle$ and $\langle R\Gamma_3$

$| \frac{d}{dR} | R\Gamma_4 \rangle$ obtained by Stern et al⁵⁾; the former is the coupling element for the crossing be-

Fig. 8 Transition moments of the radial coupling. Curve f_b is $\langle R\Gamma_3 | d/dR | R\Gamma_4 \rangle$ in ref. 5, which is the broadest one among main radial-coupling terms between adiabatic states. Curve f_a and f_c are variations of f_b . FWHM of f_a , f_b and f_c are 0.094, 0.235 and 0.47 au, respectively.

Fig. 9 Excitation functions of radial coupling for various $f_{\text{rad}}(R)$ and the emission cross section of He I $\lambda 7065\text{\AA}$ (2^3P-3^3S) line. Curve a to c are derived from f_a to f_c in Fig. 8, respectively. $\varepsilon_2: V_3$ in Fig. 2.

tween $^2\Sigma_{g0}$ of the incoming channel and $^2\Sigma_{g1}$ dissociating to He I 2^3S , which corresponds to the crossing between the diabatic curves V_0 and V_3 in figure 2. The latter is the element for the crossing, at $R=2.5$ au, between the excited levels those dissociate to He I 2^1S and to 2^3P in the separated atom limit. The curve f_c of broad width may be realized only on the crossings between the neighbouring excited levels at R of few tens au. The calculated excitation functions from these $f(R)$'s with V_3 are shown in figure 9. On highly excited level ($n \geq 3$), the radial coupling term for the crossing with the incoming channel are similar to curve a in figure 8 or may be such a curve having sharper peak than the curve a ⁵⁾ and,

Fig. 10 Excitation probability at colliding energy of 1 keV in curve b in Fig. 9.

therefore, the cross sections of direct excitation from the incoming channel probably show steep gradients near threshold energy and take maximum values at a few hundreds eV. The excitation probability P at ion energy 1 keV is shown in figure 10, as an example.

4.2 Potential energy curves of outgoing channel

The curves V_4 to V_6 in figure 2 show the potential energies ε_2 of various separation from ε_1 ; the energy difference $\varepsilon_2 - \varepsilon_1$ is proportional to $(R - R_0)$, $(R - R_0)^2$ and $(R - R_0)^4$ in curve V_4 , V_5 and V_6 , respectively, at $R < R_0$ and all the curves coincide with V_3 at $R \geq R_0$. The curve 4, 5 and 6 in figure 11 are the calculated excitation functions using V_4 , V_5 and V_6 with f_b in figure 8, respectively. The curve 7 in figure 11 indicates the excitation function for $\varepsilon_2 - \varepsilon_1 = 0$ at $R < R_0$, as a limit of approaching of ε_2 to ε_1 . The more slowly the curve ε_2 departs from ε_1 after crossing, the more rapidly the cross section increases with increasing of ion energy, and it reaches maximum at low energy as seen in figure 11.

While the variation of parameters causes considerable modification on excitation functions, we perceive general features of the radial excitation in this type of crossing, which are apparently different from the characteristics of the rotational excitation. The observed emission cross sections of He I $\lambda 7065\text{\AA}$ line ($2^3P - 3^3S$) and He I $\lambda 5876\text{\AA}$ line ($2^3P - 3^3D$) are

Fig. 11 Excitation functions of radial coupling for various ε_2 and the emission cross section of He I $\lambda 5876\text{\AA}$ ($2^3P - 3^3D$) line. Curve 4 to 6 are derived from V_4 to V_6 in Fig. 2. For curve 7, see text. $f_{\text{rad}}(R)$: f_b in Fig. 8.

shown in figures 9 and 11. The characteristics of energy dependences recognized on the cross sections agree with those of the excitation functions of the radial coupling; the cross sections increase abruptly near threshold energy and reach maximum values at low energy, compared with the cross sections of rotational excitation from the same incoming channel.

In radial excitation, the variations of $f(R)$ and of ε_2 give rise to modification of excitation functions to the same extent. Therefore, one of them at least has to be defined previously to obtain significant results from equations 2. Using the measured potential curve for the excitation process of He I 3^3D , we have determined the form of $f_{\text{rad}}(R)$ in the rough by fitting the calculated excitation function to the observed emission cross section of $\lambda 5876\text{\AA}$ line in figure 11.¹⁾

4. Conclusion

It has been shown that the rotational and radial excitations from an incoming channel through the potential crossings at small but different internuclear distances produce different types of excitation functions. It is also found that the characteristics of calculated excitation functions quite agree with the characteristic features recognized on the energy dependences of the observed emission cross sections. Then, we can estimate the type of coupling scheme of transition by considering the energy dependence of an observed emission cross section. Since the coupling scheme closely relates to populations of the magnetic sublevels of separated atoms, the determination of coupling scheme is important in studies of polarization properties of emitted light. Details of polarization effect in He⁺–He collisions will be reported in following papers.

If one of two parameters included in the coupled equations is defined previously, we can roughly estimate the form of another parameter by fitting the calculated excitation function to the profile of the measured cross section.

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References

- 1) R. Okasaka, Y. Konishi, Y. Sato and K. Fukuda : J. Phys. B: Atom. Molec. Phys. submitted.
- 2) S.H. Dworesky and R. Novick: Phys. Rev. Lett. **23**, 1484 (1969).
- 3) S.H. Dworesky, R. Novick, W.W. Smith and N. Tolk: Phys. Rev. Lett. **18**, 939 (1967).
- 4) R. McCarroll and R.D. Piacentini: J. Phys. B: Atom. Molec. Phys. **4**, 1026 (1971).
- 5) B. Stern, J. Baudon, P. Lefebure, G. Rahmat and G. Vassilev: J. Phys. B: Atom. Molec. Phys. **10**, 2165 (1977).
- 6) B. Stern, J.P. Gauyacq and V. Sidis: J. Phys. B: Atom. Molec. Phys. **11**, 653 (1978).
- 7) D.R. Bates and D.A. Williams: Proc. Phys. Soc. (London) **83**, 425 (1964).
- 8) A. Russek: Phys. Rev. A **4**, 1918 (1971).
- 9) M. Barat, S. Dhuicq, R. Francois, R. McCarroll, R.D. Piacentini and A. Salin: J. Phys. B: Atom. Molec. Phys. **5**, 1343 (1972).
- 10) R.E. Olson: Phys. Rev. A **5**, 2094 (1972).
- 11) D.R. Bates and D. Sprevak: J. Phys. B: Atom. Molec. Phys. **4**, L47 (1971).
- 12) J.S. Briggs and J. Macek: J. Phys. B: Atom. Molec. Phys. **5**, 579 (1972).
- 13) D.C. Lorents, W. Aberth and V. Hesterman: Phys. Rev. Lett. **17**, 849 (1966).