# *CROSS SECTION FOR THE EXCITATION OF* Cs II *RESONANCE LINES NEAR THE THRESHOLD OF THE* $Cs^+$ + He *REACTION THRESHOLD*

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The cross section for excitation of the Cs II resonance line emitted in the threshold region of the $Cs^+$ + He reaction is calculated theoretically in accordance with the assumption[1] that the turning and pseudo-intersection points approach each other; in this case the atomic motion must be considered quantum-mechanically. Although the kinetic energy of the atoms exceeds 100 eV it is found that the theory developed in [2] for slow atomic collisions below 10 eV can be applied. The calculation is in good agreement with experiment.

THE threshold behavior of the experimental cross section for the excitation of Cs II resonance lines in collisions between $Cs^+$ ions and He atoms has recently been studied in [1]. It was suggested that the observed effect results from intersection of the ground-state term of the $Cs^+$He quasimolecule and a term that leads to excitation of Cs II lines at 926 Å and 901 Å.[1)] This hypothesis was used as a basis for comparing the experimental data with a theoretical cross section calculated from the Landau-Zener formula. The parameters characterizing the theoretical curve were determined from the comparison:

$$U_0 = 127.5\ \text{eV},\quad \beta = 2\pi\sqrt{\mu}\,a^2 / \hbar\Delta F = 41.25\ \text{eV}^{1/2} \tag{1}$$

Here $\mu$ is the reduced mass of the colliding particles, $a \approx 1$ eV is the matrix element coupling the two terms, $\Delta F = 7.4 \times 10^{-4}$ dyn is the difference between the forces acting on the particle at $r_0$; $r_0$ and $U_0$ are the coordinates of the pseudo-intersection of the potential curves $U_{1,2}(r)$.

The discrepancy between the experimental and theoretical curves that was observed near the threshold (Fig. 1) was attributed in [1] to mutual approach of the turning and pseudo-intersection points, which is neglected in the Landau-Zener theory. A theory of nonadiabatic transitions near the turning point, in which case the quantum-mechanical character of nuclear motion must be taken into account, has been developed in [2] using a linear approximation for the terms. This situation often occurs in slow atomic collisions when the kinetic energy of relative nuclear motion is 0.1–10 eV. In the present case the kinetic energy of the colliding particles exceeds 100 eV; nevertheless, it is still possible to utilize the results obtained in [2]. This possibility is associated with the quite rapid increase in the potential energy of the $Cs^+$He system at small internuclear separations ($r \sim 10^{-8}$ cm). It is therefore entirely possible to have a situation where the de Broglie wavelength is comparable with the size of the region $\delta r$ in which a nonadiabatic transition occurs and the theory of [2] can be applied, although outside this region nuclear motion may be analyzed classically.[2)]

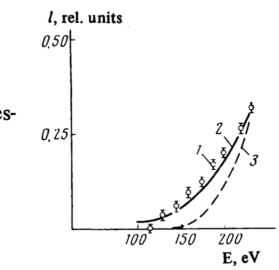


FIG. 1. 1—experimental points; 2—present calculation; 3—curve calculated from the Landau-Zener formula.

It was shown in [2] that the probability $w(\rho)$ of a nonadiabatic transition for $l = 0$ depends on two dimensionless parameters $\epsilon$ and b, and an analytic form of $w(\rho)$ is obtained for certain regions of $\epsilon$ and b:

$$\varepsilon = E_0\Delta F / 2aF, \quad b = 4a\sqrt{\mu a} / \hbar\sqrt{F\Delta F},$$
$$E_0 = E_\infty - U_0, \quad F = (F_1F_2)^{1/2}, \quad F_{1,2} = -\left.\frac{\partial U_{1,2}(r)}{\partial r}\right|_{r=r_0}, \tag{2}$$

where $F_1$ and $F_2$ are the forces at the intersection point of zeroth approximation terms.

To determine the cross section we must know the transition probabilities for different values of $l$. We may use the procedure suggested by Kotova.[3] A centrifugal term appearing for $l \neq 0$, and its first derivative at the intersection point $r_0$, are added to $E_0$ and F as given for $l = 0$, i.e., in (2) we must replace $E_0$ and F by

$$E_0' = E_0 - \frac{\rho^2}{r_0^2}E_\infty, \quad F' = (F_1'F_2')^{1/2}, \quad F_{1,2}' = F_{1,2} + \frac{2E_\infty}{r_0^2}\rho^2. \tag{3}$$

However, this procedure is not entirely correct, since the system of equations for $l = 0$ in the case of linearly approximated terms possesses no singularity at zero and can therefore not serve as a standard for the case of arbitrary $l$. The aforementioned substitution can be performed only when the centrifugal term

1) It is difficult to analyze the terms of this system in detail because of insufficient experimental and theoretical information.

2) Specifically, when calculating cross sections we can replace summation over the orbital quantum number $l$ by integration over the impact parameter $\rho$.

produces no more than a small deviation from linearity in the transition region, i.e., only subject to the condition

$$\frac{r_0 F}{2E_\infty} \gg \frac{\rho^2}{r_0^2} \text{ or } \frac{U_0}{2E_\infty} \gg \frac{\rho^2}{r_0^2}. \quad (4)$$

If we ignore this condition and assume (3) for any $\rho$ we arrive at an incorrect value for the transition probability.[3)] Thus for large $\rho$ we have $b \sim \rho^{-1}$ and for the transition probability we can use

$$w(\rho) = \pi b^{4/3} \Phi^2(-\varepsilon b^{2/3}), \quad (5)$$

which was obtained by Nikitin[4] for small b; $\Phi$ is an Airy function. The final result is $w(\rho) \sim \rho^{-1/3}$, which is entirely incorrect, since it leads to a divergent cross section.

It seems reasonable, therefore, to calculate the cross section from

$$\sigma(E_\infty) \geqslant 2\pi \int_0^{\rho_{max}} w[\varepsilon(\rho), b(\rho)] \rho \, d\rho, \quad (6)$$

where $\rho_{max}$ is determined by satisfying (4), while $\epsilon$ and b are obtained from (2) and (3). To evaluate the cross section from this equation we must know $w(\rho)$ on the portion of the $\epsilon(\rho)$–$b(\rho)$ curve that corresponds to $\rho \leq \rho_{max}$. It follows from (2) and (3) that this curve is a parabola and that the indicated portion may go through regions where analytic expressions for the probability $w(\rho)$ do not exist.[2]

We plan a calculation of the cross section using (6) by integrating numerically a system of differential equations for the purpose of obtaining $w(\rho)$ in wide ranges of $\epsilon$ and b.

By analyzing the region of difference between the experimental and theoretical cross sections ($E_\infty \leq 225$ eV) we obtain $\epsilon_0 = \epsilon(\rho = 0) = 1$ and $b_0 = b(\rho = 0) = 4.1$ corresponding to the energy region ($\approx 225$ eV) where the Landau–Zener formula ceases to describe experiment satisfactorily and we must allow for the theoretical effects predicted in [2].

It is shown by a comparison of our Fig. 2 with Fig. 1 of [2], which shows the location of the regions where an analytic expression for $w(\rho)$ exists, that to calculate the cross section in the studied case we may use the following equation for the transition probability:

$$w(\rho) = 2 \exp[-b\Delta(\varepsilon)]. \quad (7)$$

The function $\Delta(\epsilon)$ is tabulated in [2] for $-2 < \epsilon < 3$; however, the value of the integral in (6) is derived mainly from the region $\epsilon > 0$ (suprabarrier transitions for $E_\infty > 127$ eV). In this region $\Delta(\epsilon)$ can with good accuracy be represented as follows:[4]

[3)]We note that (3) is used legitimately in [3], where no essential use is made of the dependence on $l$ that is found in the modulus of the transition probability, and the phase is assumed to be small compared with the quasiclassical case.

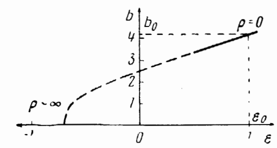


FIG. 2. Values of $\epsilon$ and b for which $w(\rho)$ must be known at $E_\infty = 225$ eV; the dashed segment corresponds to the region of $\rho > \rho_{max}$.

$$\Delta(\varepsilon) = 1.23 - 0.86\,\varepsilon. \quad (8)$$

To calculate the cross section we expand $\epsilon$ and b in powers of $\rho$ up to $\rho^2$ in the vicinity of $\rho = 0$, which is entirely permissible for $\rho \leq \rho_{max}$, and we substitute (7) and (8) in (6). In using (6) to evaluate the cross section we assumed $\rho_{max}^2/r_0^2 = r_0F/4E_\infty$, which is somewhat arbitrary. However, it follows from the calculation that when we expand $\epsilon$ and b in powers of $\rho$, i.e., we assume that head-on collisions make the main contribution to the cross section, the result is practically independent of our choice of $\rho_{max}$ for $E_\infty \geq U_0$ and depends only slightly on $\rho_{max}$ for $E_\infty < U_0$.

The abscissa $r_0 \approx 0.65 \times 10^{-8}$ cm of the pseudo-intersection was obtained for $Cs^+He$ ($U_0 = 127.5$ eV) from Firsov's familiar equation in [5]. The results of the calculation, shown in Fig. 1, agree quite well with experiment.

The integral in (6) can be evaluated differently. Since $\epsilon/E_0'$ and b are only weakly dependent on $\rho$, we can here change the integration over $\rho$ to integration over $\epsilon$, assuming b = const (the straight line in Fig. 2). However, the agreement between the calculated and experimental curves is diminished in the process.

We note, finally, that (6), (7), and (8) yield approximately $3 \times 10^{-18}$ cm² as the absolute cross section for Cs II $\lambda = 926.7$ Å in the case of $E_\infty = 225$ eV.

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