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# Cesium Resonant Total Charge-Transfer Cross Section and Oscillatory Structure*

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A more detailed measurement and calculation are reported for the $Cs^{+}+Cs$ charge-transfer cross section which contains continuous uniform oscillatory structure. Ten oscillation maxima are experimentally observed in the energy range from 0.6 to 21 keV. The oscillations are regular with inverse velocity and appear to show two superimposed oscillation frequencies. Calculations suggest that this may be due to the combined effect of a maximum in the interaction potential difference and of a large repulsive electron core, each generating a separate oscillation. It is shown that there is a very wide range of different potentials which could explain the oscillations.

## INTRODUCTION

Several measurements of the Cs resonant total charge-transfer cross section have been made during the past decade with most of the results reported in literature in fairly good agreement. The earlier measurements[1-4] show the typical smooth variation of the resonant cross section ($\sigma$) with the relative velocity given by $\sigma^{1/2}=A-B\ln v$. More recent measurements show this cross section to contain oscillatory structure.[5,6]

Smith[7] subsequently showed that such oscillations can result from a stationary phase effect if the difference between the gerade and ungerade phase shifts passes through a maximum. This may occur in either of two ways: the interaction potential difference may pass through a maximum (potential maximum oscillations)[7] or the two potentials may have a strong repulsive core (core oscillations).[8] Oscillations resulting from a maximum were obtained in the calculations of Peek *et al.*[9] for $Li^+$ – Li collisions using an *ab initio* calculation of the two lowest $Li_2^+$ potential curves. The potential difference has a maximum because the gerade and ungerade potential curves cross at small internuclear distances. The calculated and subsequent experimental cross sections for this case are in very good agreement.[10] A detailed explanation of Smith's stationary phase theory is given by Perel[11] using the Li resonant cross sections as an example. A method of adjusting the interaction potential parameters to get agreement between theory and experiment has been used recently by Olson[12] to calculate the oscillatory structure in $Rb^+$ – Rb and $Cs^+$ – Cs collisions.

The present work describes more careful measurements and calculations of $Cs^+ + Cs$ charge transfer designed to examine the oscillatory structure in more detail. Ten oscillation maxima were experimentally observed over an energy range from 0.6 to 21 keV. The oscillations are regular with inverse velocity in agreement with theory; they appear to show two overlapping oscillations, one of which may be due to a maximum in the potential difference and the other due to the repulsive core.

## EXPERIMENTAL RESULTS

The measurement technique, described previously,[5] utilized a modulated crossed beam technique with phase-sensitive detection and surface ionization to generate the ions and detect the atoms. Data were taken by directly plotting the relative cross section versus the ion acceleration voltage on an *XY* recorder using a log multiplier circuit to obtain the ratio of the charge-transfer signal to the ion-beam current.[13] The resulting plot is then correlated with absolute data points to give absolute cross sections.

Figure 1 shows the results of the recent measurement of the cross section as a function of the ion velocity. Oscillatory structure is evident upon the averaged cross-section curve which decreases with increasing ion velocity. The oscillatory amplitude and width generally increases with increasing velocity. The positions of the oscillations are slightly shifted from the earlier measurement[5] where only $2\frac{1}{2}$ oscillations were observed. This may have resulted from the data taking and reduction technique employed with the earlier measurements.

The absolute values of the present experimental cross sections are estimated to be uncertain to within ±10%. The plotting technique provided a greater certainty in the position of the oscillation with oscillation amplitudes of 1% of the cross-section value discernable, but uncertain by about a factor of 2. The data below 1 keV are less reliable because the decrease in ion-beam current at the low-voltage end of the measured range resulted in lower signal-to-noise ratios.

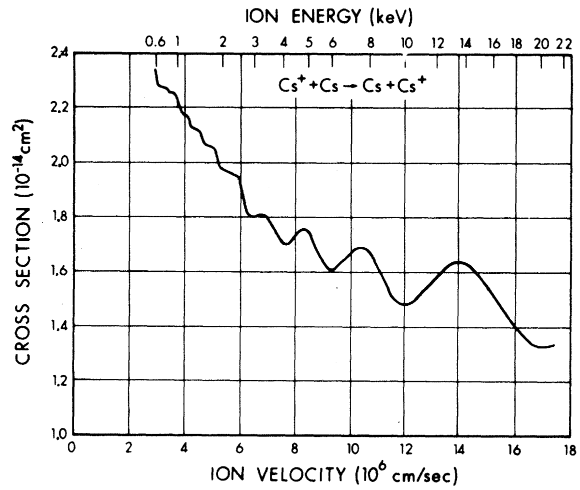


FIG. 1. Results from recent measurements of Cs resonant charge-transfer cross sections shown as a function of the ion velocity and energy. These cross sections are similar to the previous determination (Ref. 5) except that more oscillatory structure has been uncovered.

## CORRELATION WITH THEORY

It has been shown by Smith[7] that when the potential difference passes through a maximum the cross section ($\sigma$) can be expressed as

$$\sigma = \bar{\sigma} - \alpha(v)\cos(\pi\beta v^{-1} - \delta), \qquad (1)$$

where $\bar{\sigma}$ is the mean cross section, $\alpha(v)$ is the oscillation amplitude (proportional to $v^{1/2}$), and $\delta$ is a phase constant equal to $\frac{1}{4}\pi$. When the potential difference has no maximum and the oscillations are due to the central core, Eq. (1) is still approximately valid with $\delta$ no longer equal to $\frac{1}{4}\pi$, but tending to decrease in value, becoming negative as the repulsion of the core increases.

To determine the experimental values of the oscillation frequency $\beta$ and the phase constant $\delta$ given in Eq. (1), cross-section maxima and minima are related to the integer multiplier of $\pi$ by setting $n = (\pi\beta^{-1} - \delta)$. Odd and even multiples of $\pi$ represent maxima and minima on a plot of $n$ versus $v^{-1}$ (Fig. 2) with the slope equal to $\pi\beta$ and the ordinate intercept equal to $\delta$. Note that $\delta$ is ambiguous by a value of $2\pi$. The straight line shown in Fig. 2 yields $\beta = 0.83 \times 10^8$ cm/sec based on the high-energy (low-inverse velocity) data points which are considered more reliable. The phase $\delta$, found to be approximately $-\pi$, is less accurately determined because it is an extrapola-

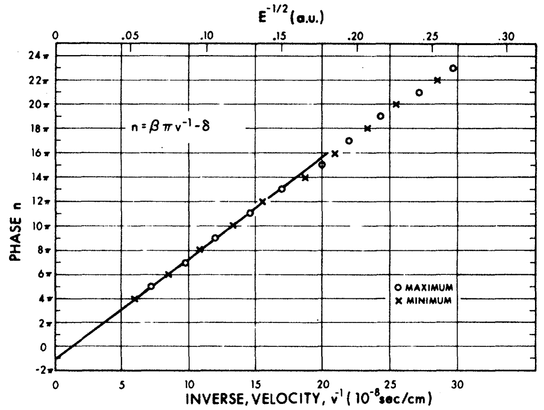


FIG. 2. Plot of the experimental oscillation maxima and minima using inverse velocity coordinates. The slope of the line is $\pi\beta$, the oscillation frequency and the ordinate intercept is the phase constant $\delta$ which is uncertain by multiples of $2\pi$.

tion of the experimental results as illustrated in Fig. 2. If the oscillations are due to a potential maximum, $\delta$ should be $\frac{1}{4}\pi$ and a discrepancy of either $\frac{3}{4}\pi$ or $\frac{5}{4}\pi$ exists. This seems to be larger than the possible combined experimental and extrapolated errors.

Similar discrepancies were obtained for other alkali metal resonant measurements[14,15] indicating that the core effect does occur, or has, at least, an influence on the oscillation phase constant. This is true especially for heavy atoms and for excited states when the core is most repulsive. One effect which can cause a phase shift is rotational coupling of the ${}^2\Sigma_u^+$ state with higher states,[16] but in our case the velocity appears to be too low for this to be important.

Two pairs of potential curves were constructed to illustrate both potential maximum oscillations and core oscillations and for comparison with the experimental results. Figure 3 shows the gerade potential ($V_g$) for the case of a potential difference maximum (curve I) and the case of a highly repulsive electron core (curve II). Figure 4 shows potential difference ($\Delta V$) curves illustrating a maximum (curve I) and a case of a repulsive core (curve II). The monotonic decrease in curve II is a form commonly seen for other molecular ions such as $H_2^+$, $He_2^+$, etc. In these latter cases, small amplitude oscillatory structures have been calculated which are presumably due to the (small) core effect.

When the potential difference has a maximum, then the phase difference has the form shown in Fig. 5. The flat region at very small impact parameters is due to the core and it causes one type

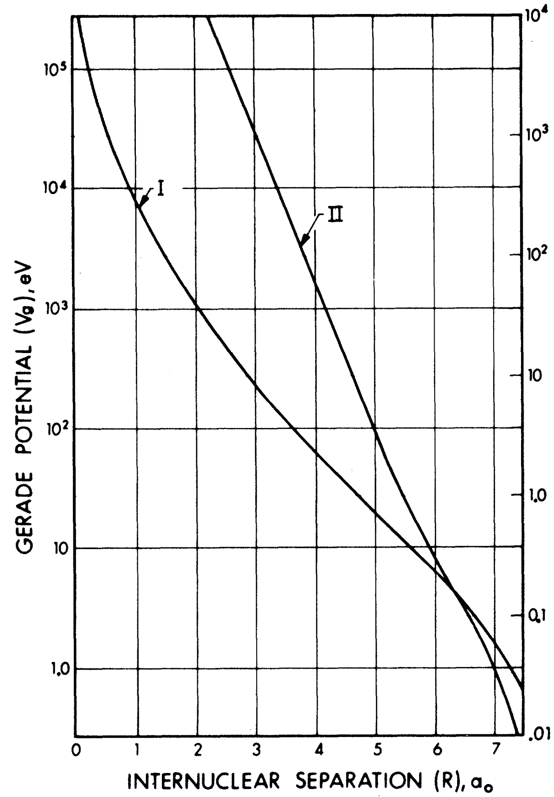


FIG. 3. Gerade potentials I and II used to generate calculated cross sections containing oscillations. Note that potential II has the highly repulsive core.

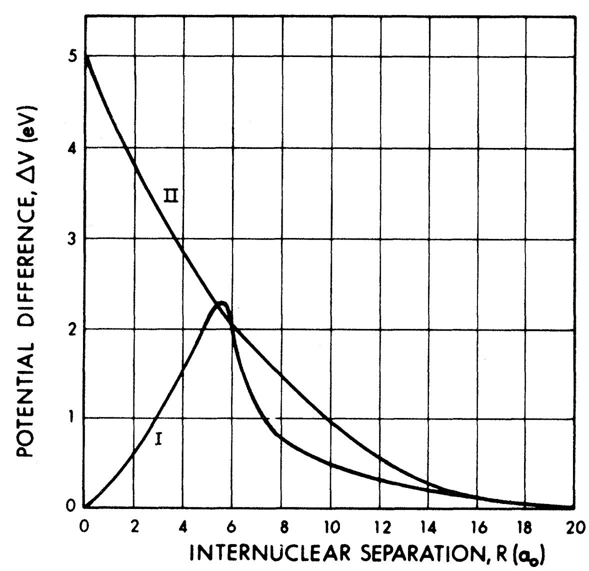


FIG. 4. Potential difference curves I and II used to generate calculated cross sections containing oscillations. Note that curve I has a maximum.

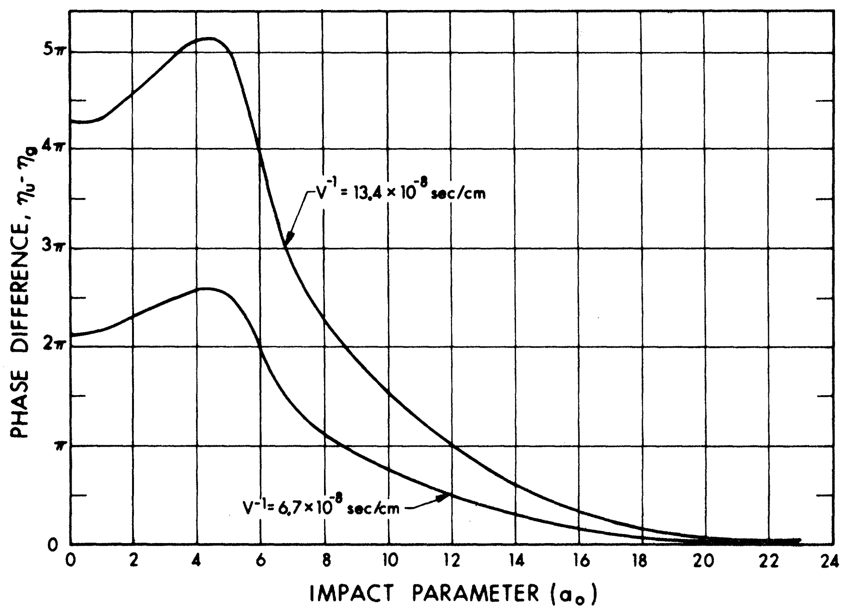


FIG. 5. Plot of the phase difference $\eta_u - \eta_g$ for potential I as a function of impact parameter for two inverse velocities.

of oscillation to occur. The maximum in the phase difference is due primarily to the potential maximum and causes another type of oscillation. At high energy ($v^{-1} = 6.7 \times 10^{-8}$ sec/cm in Fig. 5) the two amplitudes of these oscillations reinforce one another. At a lower energy ($v^{-1} = 13.4 \times 10^{-8}$ sec/cm in Fig. 5) destructive interference occurs and the amplitude decreases because the stationary phases differ by about $\pi$. A drop in amplitude in both the theoretical (potential curve I) and experimental cross sections near $v^{-1} = 15 \times 10^{-8}$ sec/cm is apparent in Fig. 6 which shows the cross section versus inverse velocity. At lower energies the amplitudes reinforce one another and an increase in the amplitude occurs.

Even when the potential difference has no maximum, the phase difference still has the form shown in Fig. 5. As a result, the core effect also gives rise to a pair of oscillation frequencies. This is apparent from the theoretical results shown in Fig.

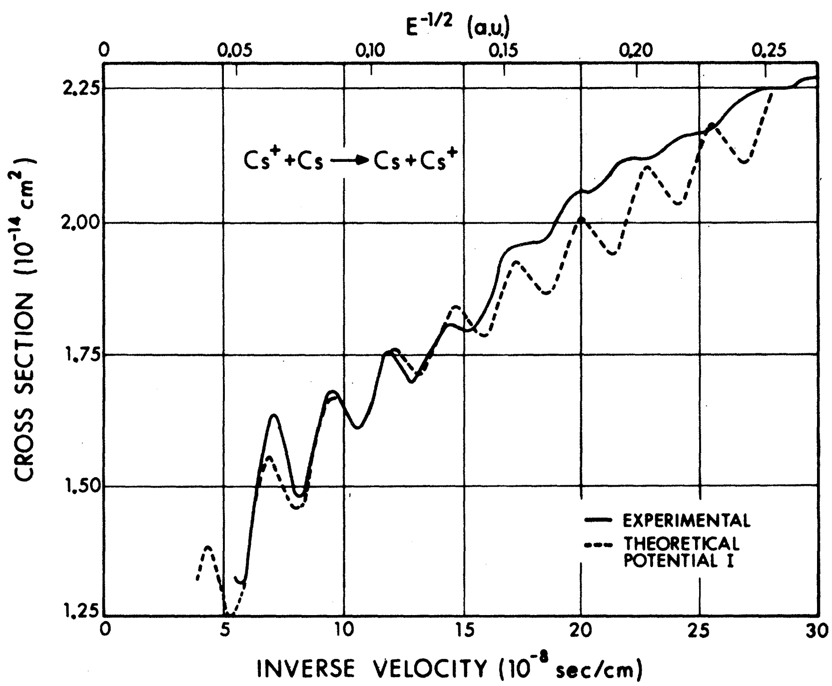


FIG. 6. Comparison of the experimental and the calculated cross sections on inverse velocity coordinates. The calculations were based on gerade potential curve I shown in Fig. 3 and potential difference curve I of Fig. 4 which contains a maximum.

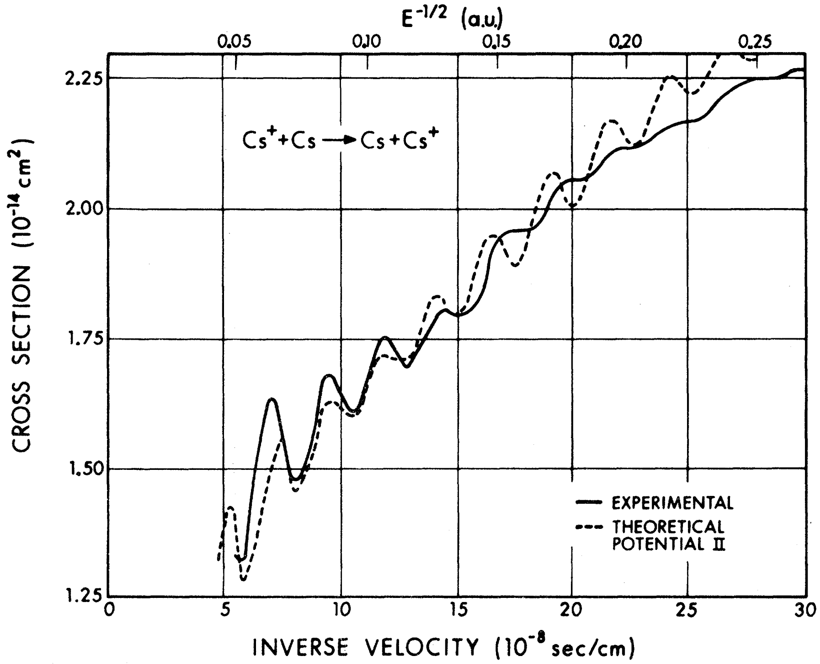


FIG. 7. Comparison of the experimental with the calculated cross section II on inverse velocity coordinates. These calculations were based on the curves labeled II, also shown in Figs. 3 and 4, which contain a highly repulsive electron core.

7 obtained using potential II.

Finally, we must stress that the two potential differences in Fig. 4 are by no means unique. Given any form of potential difference with a maximum $[\Phi(R)]$ we first express it as

$$\Delta V(R) = \epsilon\Phi(R/\gamma)\,, \tag{2}$$

where initially $\epsilon = 1$ and $\gamma = 1$ and we calculate the cross sections. Then, by a comparison with experimental results and dimensional analysis, if we need to increase the wavelength $[\Delta(1/v)]$ between maxima by a factor $\lambda$ and to increase the amplitude of the oscillations by a factor $A$ we equate

$$\gamma = \lambda^{-1/4} A^{1/2} \text{ and } \epsilon = \lambda^{-3/4} A^{-1/2}. \tag{3}$$

By this method a set of oscillations almost identical to those in Fig. 6 can be produced for any form of potential difference with a maximum.

The formulas in Eq. (3) are only approximate when applied to core oscillations, but they can be used iteratively for almost any form of potential without a maximum. Hence, the number of potentials which can generate the oscillations is bewildering.

One result of these analyses is that these oscillations should be extremely common for resonant and nonresonant charge transfer and for excitation cross sections. Another result is that it does not appear to be possible to uniquely determine the pair of appropriate potentials from total cross sections alone. Differential cross sections are also needed.


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# Cross Sections for Energy Transfer in Classical Coulomb Collisions

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The cross section $Q(U)$ for energy transfer of at least $U$ is given for the case where the incident particle is lighter than the target particle. Complete results for $Q(U)$ are represented with the aid of a diagram, the coordinates of which are nondimensionalized mass and nondimensionalized energy of the target particle. Some remarks are made about scaling laws for direct excitation.

## I. INTRODUCTION

Classical methods for calculating energy-transfer cross sections have recently found wide application in the estimation of inelastic atomic- and molecular-collision cross sections. The idea of using classical methods for this purpose is due to Thomson.[1] His method consists of calculating the cross section $Q(U)$, for which an incident charged particle transfers an amount of energy of at least $U$ to a stationary electron. This cross section is taken to give the cross section for ionization of an atom or molecule, with the $U$ set equal to the ionization energy of the orbital electron to be removed. Thomson's results were extended by Gryziński,[2-5] who took account of the orbital motion of the atomic electrons, and who emphasized the agreement with experiment which could be obtained by making a number of semi-empirical approximations (cf. also, Ref. 6).

A further extension was made by Gerjuoy,[7] who calculated the differential energy cross section $\sigma(U) = -(d/dU)Q(U)$ for an arbitrary mass ratio of the collision partners. The result for $\sigma(U)$ in the special case of an incident particle having a mass $m_2$ much larger than the mass $m_1$ of the target particle was also given by Vriens.[8] Expressions for the cross section $Q(U)$ for the special case $m_1 = m_2$ were given in Refs. 9–12 and for the case $m_1 \leqslant m_2$ in Ref. 13.

In the present paper we extend the calculations of Refs. 2–13 by obtaining the results for the cross section $Q(U)$ when $m_1 > m_2$. These results are of interest in view of the equality of the quantum-mechanical and classical Coulomb cross sections. So far, no applications have been found of either the results for $Q(U)$ or the previously given results for $\sigma(U)$ when $m_1 > m_2$.

## II. RESULTS FOR $Q(U)$ FOR ARBITRARY RATIO $m_1/m_2$

The situation considered is sketched in Fig. 1. A target particle (called field particle in Refs. 2–5) of mass $m_1$ and velocity $\vec{v}_1$ is suffering a collision with an incident particle (called test particle in Refs. 2–5) of mass $m_2$ and velocity $\vec{v}_2$. That the target particle may be part of an atom is ignored in evaluating the consequences of the collision. The force between the two particles is assumed to be conservative, and derivable from a spherically symmetric potential. It is possible to calculate the amount of energy transferred from the incident particle to the target particle in the laboratory frame of reference as a function of the impact parameter $b$, and of other variables

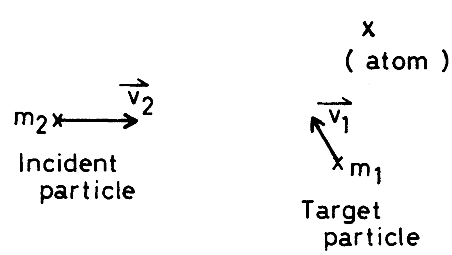


FIG. 1. Particles before collision.