Angle-differential and momentum-transfer cross sections for e^{-}+Rb, Cs, and Fr collisions at low energies: $^{3}F^{o}$ shape resonances in Rb^{-}, Cs^{-}, and Fr^{-} ions

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Based on the relativistic Dirac *R*-matrix method, we calculate angle-dependent and momentum-transfer cross sections for electron scattering by Rb, Cs, and Fr atoms at impact energies below 3 eV. Our results for momentum transfer for e^{-}+Rb and Cs collisions are compared with available data from swarm experiments. We find clear evidence for a $Cs^{-}(^{3}F^{o})$ shape resonance at 1.528 eV, in excellent agreement with angle-dependent electron-scattering measurements. We analyze and compare the $^{3}F^{o}$ shape resonance in e^{-}+Rb, Cs, and Fr elastic collisions.

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I. INTRODUCTION

For several decades, negative ions have attracted much interest from both theorists and experimentalists and are the subject of recent reviews [1–4]. Nevertheless, the spectra of many negative ions have not been investigated in detail. Recently, we have analyzed the $^{3}P^{o}$ shape [5] and the $^{3}P^{e}$, $^{1}P_{1}^{o}$, and $^{1}D_{2}^{o}$ Feshbach resonances [6] below the first $np_{3/2}$ excitation threshold ($n=5$ for Rb, 6 for Cs, and 7 for Fr) for slow electronic collisions with Rb, Cs, and Fr atoms in partial and total cross sections. The calculations in [5,6] are based on the Dirac *R*-matrix method [7] and agree well with various experiments and other nonrelativistic calculations. In this paper, we extend our studies to the $^{3}F^{o}$ shape resonances in Rb^{-}, Cs^{-}, and Fr^{-} ions in elastic angle-integrated cross section. Particular attention will be devoted to the $^{3}F^{o}$ shape resonance of Cs^{-} observed at about 40 meV above the $6p_{3/2}$ detachment threshold in elastic angle-differential measurements for electron scattering by Cs atoms by Gehenn and Reichert [8], but never confirmed in previous angle-differential cross section (DCSs) calculations at the same energy. The measurements of Gehenn and Reichert are still being used as benchmark results for other experimental and theoretical studies of low-energy electron scattering by Cs atoms (see, e.g., the studies on spin asymmetries in [9]).

Our present calculations are based on the suite of the relativistic Dirac *R*-matrix programs of Thumm and Norcross [7], which provides electron-impact scattering data within an effective two-electron model in which the valence and scattered electrons of the electron-alkali atom system move in the field of a polarizable noble-gas-like core. The model potential we are using to describe the electrostatic interaction between the projectile electron and the atomic targets (Rb, Cs, and Fr) was discussed in [5]. We analyze the collision using the *R*-matrix procedure described in [5,6]. The scattering amplitudes and cross sections are computed from the energy-dependent **K** matrix by using the Dirac *R*-matrix method [7] and the same jj-recoupling scheme between the angular momenta of the scattered electron and the target valence electron as Thumm and Norcross [10]. The major difference with respect to the electron-Cs scattering calculations in [10] is that in the present computations for Rb, Cs, and Fr targets we use the experimental atomic excitation energies instead of theoretical values and more continuum orbitals. In the present calculations we include the first five bound states of the target: $ns_{1/2}$, $np_{1/2}$, $np_{3/2}$, $(n-1)d_{3/2}$, $(n-1)d_{5/2}$ (with $n=5$ for Rb, 6 for Cs, or 7 for Fr), and 28 continuum orbitals for each angular momentum l up to $l_{max}=12$. This guarantees convergence of the total integrated cross sections (TCSs) for collision energies below 3 eV. However, the elastic DCSs converge much slower with l_{max} than the TCSs. We therefore include partial waves for $l_{max}\leqslant l\leqslant 50$ in our converged DCS calculations (cf. Ref. [10]), by using the effective range formula of O'Malley, Spruch, and Rosenberg [11].

This paper is organized as follows. In Sec. II, we explain our theoretical results for angle-differential and momentum-transfer cross sections for e^{-}+Fr collisions at low energies, and compare our data for momentum transfer for Rb and Cs atoms with results in swarm experiments. In Sec. III, we discuss the $^{3}F^{o}$ resonance for Rb^{-}, Cs^{-}, and Fr^{-} ions and the influence of relativistic interactions. In addition, we compare our $^{3}F^{o}$ resonance for Cs^{-} with accurate angle-dependent experimental data. Unless otherwise indicated, we shall use atomic units.

II. ANGLE-DEPENDENT AND MOMENTUM-TRANSFER CROSS SECTIONS

A. Angle-dependent cross sections in e^{-}+Fr collisions

Figure 1 shows our theoretical elastic DCS results for e^{-}+Fr collisions at energies E below 3 eV and for scattering angles θ between 0° and 180°. The dependence in E and θ of the DCS is similar for all three targets. Therefore, we focus on DCS results for e^{-}+Fr collisions. Theoretical DCS results for e^{-}+Cs collisions in the same energy range have been published in Ref. [10]. In general, the magnitude of the elastic DCS decreases smoothly with E for a fixed scattering angle, except for energies very close to resonance states [Fig. 1(a)] and threshold singularities [Fig. 1(b)]. Figure 1(a) shows the $^{3}P^{o}$ shape resonance of Fr^{-}, which was recently investigated in TCS for e^{-}+Fr collisions (see Fig. 2 in Ref. [5]). The Fr atom is more complex than Rb and Cs atoms, and its electronic structure is more strongly influenced by

