Singularities in ECPSSR Cross Sections

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Perturbed stationary state theory with corrections for energy loss, Coulomb deflection, and relativistic effects (referred to as the ECPSSR theory [1]) is routinely used to calculate the cross sections for K-shell vacancy production by direct ionization in collisions between stationary target atoms and fast heavy-ion projectiles. It is based on the plane-wave Born approximation (PWBA), but it takes into account the Coulomb deflection of the projectile, the recoil of the target atom, the increased binding of the target K-shell electrons due to the projectile nuclear charge, and the polarization of the electrons in the target atoms. The ECPSSR formulation is non-relativistic, but it incorporates corrections for relativistic effects.

The region of proven validity of the ECPSSR formulation originally covered the region defined by the parametersZ_1 / Z_2 ranging from 0.03 to 0.3 and v_1 / v_{2K} between 0.07 and 2, where Z_1, Z_2, v_1, and v_{2K} are, respectively, the atomic numbers of the projectile and target, and the velocities of the projectile and the K electron of the target. This region has been extended to include the collision systems with Z_1 / Z_2 from 0.02 to 1.4 and v_1 / v_{2K} up to 3.2 [2]. On the other hand, experiments with 10 MeV/u beams ranging in atomic number from Ne ($Z_1 = 10$) to Bi ($Z_1 = 83$), colliding with solidCu [3] and Al [4] targets ($Z_2 = 29$ and 13, respectively), revealed that the discrepancies between theory and experiment were even larger for ECPSSR theory than for PWBA.

This unexpected result lead to the discovery of a range of singularities originating from the ECPSSR correction for binding and polarization effects (i.e., the perturbed stationary statecorrection).Namely, according to the PWBA formulation, the reduced (universal) cross section for ionization of a target-atom electron is a function of the reduced projectile energy η and the reduced target-electron binding energy θ [5]. In the ECPSSR theory [6], θ is replaced with a product of θ and the correction factor ζ_K [eq.(45) in Ref. 6]. However, it was found that for certain combinations of the collision parameters, the value of ζ_K passes through zero and becomes negative. As a result, the calculated cross section for ionization of the target electron becomes infinite and then changes sign.

The correction parameter ζ_K is defined by the expression

$$\zeta_K = 1 + \frac{2\, Z_1\, [B(\xi) - H(\theta,\xi)]}{(Z_2 - s_2)\, \theta} , \qquad (1)$$

where s_2 is the Slater screening constant for the target K electron [equal to zero for a hydrogen target ($Z_2 = 1$) and 0.3 for other targets]. The θ parameter is given by

$$\theta = \frac{E_B(Z_2)}{E_B(1)\ (Z_2 - s_2)^2}\ , \qquad (2)$$

where $E_B(Z_2)$ is the binding energy of a K electron in target with atomic number Z_2,

$$\xi = 2\ \frac{\sqrt{\eta}}{\theta}\ , \qquad (3)$$

$$\eta = \frac{R_{ep}}{(Z_2 - s_2)^2}\ \frac{E_1}{E_B(Z_2)}\ , \qquad (4)$$

E_1 is the projectile kinetic energy and R_{ep} is the electron to proton mass ratio. B and H are rather complicated functions of ξ [6].

The projectile energies and target atomic numbers for which $\zeta_K = 0$ [according to eq.(1)] is shown in Figure 1 for Bi, Xe, and Kr projectiles. The regions inside the loops correspond to negative values of ζ_K and negative cross sections. The regions just outside the loops correspond to the cross sections that are expected to be significantly overestimated.

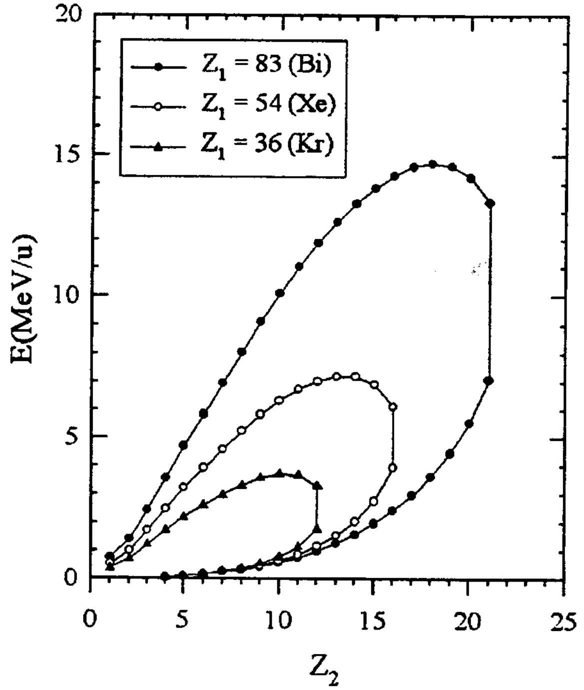

Figure 1. Collision systems corresponding to singularities in the ECPSSR theory.

References

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