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Theoretical state-selective and total cross sections for electron capture from helium atoms by fully stripped ions

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ABSTRACT

The four-body boundary-corrected first Born (CB1-4B) approximation is used to compute cross sections for single electron capture from helium targets by fully stripped ions. The projectile ions are H^+, He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+}, O^{8+}, and F^{9+}. An extensive list of theoretical state-to-state cross sections in these collisions at energies ranging from 20 to 10 000 keV/amu is given. This list includes the state-selective cross sections Q_{nlm} for each individual triple of the usual quantum numbers $\{n, l, m\}$ of the final hydrogen-like states alongside Q_{nl} and Q_n for the pertinent sub-shells and shells where the respective summations over m and $\{l, m\}$ have been carried out. The maximal value of the principal quantum number n was chosen to vary from 4 (H^+) to 10 (F^{9+}) so as to satisfy the condition $n \geq Z_P$, where Z_P is the nuclear charge of the projectile. Usually, the largest cross sections stem from those values of n that match the projectile charge ($n = Z_P$). The total cross sections for capture summed over all the quantum numbers $\{n, l, m\}$ are also tabulated. The overall goal of this study is to fill in lacunae in the existing databases of charge exchange cross sections that are needed in several inter-disciplinary fields. For example, in particle transport physics, which is of utmost importance in such emerging branches as hadron therapy, these cross sections constitute a part of the multifaceted input data for stochastic simulations of energy losses of multiply charged ions in matter, including tissue. Other significant uses of the present data are anticipated in charge exchange diagnostics within thermonuclear research project as well as in applications covering the relevant parts of plasma physics and astrophysics.

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Contents

1. Introduction

The present work is focused on a single electron capture from helium atoms interacting with completely stripped ions as projectiles (H^+, He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+}, O^{8+}, and F^{9+}), with all four particles actively participating in the collisional events. The prior version of the CB1-4B approximation is employed to compute state-selective and total cross sections. The CB1-4B method is a fully quantum-mechanical four body formalism, since it explicitly considers each individual particle and all the interactions among them in the collision under study. The CB1-4B model preserves the correct boundary conditions in both collisional channels. It is well-known that the problem of the correct Coulomb boundary conditions, or equivalently, the asymptotic convergence, or the asymptotic freedom [1–4] is of essential importance for atomic and molecular collisions.

In our previous work [5], the generalization of the CB1-4B theory has been carried out to single electron capture by a bare projectile from a helium-like atomic system into the final *arbitrary* shells $\{nlm\}$ of the transferred electron. Subsequently, the CB1-4B method was successfully applied [6] to a single electron capture from helium atoms by He^{2+}, Be^{4+}, B^{5+} and C^{6+} ions. Detailed comparisons with a number of measurements [5,6] show that theoretical cross sections from the CB1-4B approximation are in a reasonable agreement with the available experimental data.

Electron capture into excited states is expected to play an important role, at least at lower and intermediate energies. Information about the sub-shell populations of states formed by charge exchange is important in a number of applications in plasma physics, astrophysics, thermonuclear fusion research and medical accelerators for hadron radiotherapy. For the relevance of the CB1-4B formalism to different interdisciplinary application, see for example Ref. [5]. Due to great computational difficulties in treating four body systems, such as collisions of bare ions with helium target, an independent electron model has been often adopted in many theoretical studies of electron capture processes. In such collisions, the captured electron is assumed to move in an averaged Coulomb potential field with an effective nuclear charge. The CB1-4B theory goes beyond the usual independent-particle frozen-core approximations and obeys the asymptotic convergence criteria of Dollard [1–4,7,8] for Coulomb potentials.

The post transition amplitude of the CB1-4B model for single charge exchange has been derived in Ref. [9] in terms of five-dimensional integrals over real variables. Further, Ref. [5] has reported on an alternative semi-analytical reduction of the prior form of the T-matrix elements from the CB1-4B method yielding computationally more efficient two-dimensional quadratures. On the other hand, the computations show [9] that prior and post cross sections (both state-selective and total) of the CB1-4B approximation with the inclusion of the complete perturbation potentials V_i and V_f are nearly identical. This is an excellent property of the CB1-4B method, since the same physical assumptions are involved in the prior and post forms of this theory. Due to the above-mentioned properties of the CB1-4B model, the prior version is more convenient in the applications and this is the reason for using the prior form in the present computations.

With regard to our previous studies [5,6], we presently provide a comprehensive set of new theoretical results for N^{7+}, O^{8+}, and F^{9+} ions on helium target. Simultaneously, for the other considered ions colliding with helium the energy intervals are substantially extended.

Atomic units will be used throughout this paper unless otherwise stated.

2. Theory

Detailed computations for the following charge exchange reaction:

$$X^{Z_P+} + He(1s^2) \longrightarrow (X^{Z_P+}, e)_{nlm} + He^+(1s)\,, \tag{1}$$

are carried out with $Z_P = 1 - 9$, where Z_P is the charge of the projectile nucleus and nlm is the usual set of three hydrogen-like quantum numbers, whereas the parentheses in $(X^{Z_P+}, e)_{nlm}$ denote the bound state.

The prior form of the transition amplitude for process (1) in the CB1-4B approximation reads as [5]:

$$T_{if}(\vec{\eta}\,) = \int\int\int \mathrm{d}\vec{x}_1 \mathrm{d}\vec{x}_2 \mathrm{d}\vec{R}\varphi^*_{nlm}(\vec{s}_1)\varphi^*_{\mathrm{T}}(\vec{x}_2)[V(R,s_1)+V(R,s_2)] \times \varphi_i(\vec{x}_1,\vec{x}_2)\,\mathrm{e}^{-i\vec{\alpha}\cdot\vec{R}-i\vec{v}\cdot\vec{x}_1}(vR+\vec{v}\cdot\vec{R})^{i\xi}\,, \tag{2}$$

$$V(R,s_i) = \frac{Z_P}{R} - \frac{Z_P}{s_i}, \quad (i=1,2), \tag{3}$$

with $\xi = (Z_P - 1)/v$, where v is the velocity of the projectile. Here $\vec{s}_1$ and $\vec{s}_2$ ($\vec{x}_1$ and $\vec{x}_2$) are the position vectors of the captured and non-captured electron (e_1 and e_2) relative to the nuclear charge of the projectile (target nucleus). Further, let $\vec{R}$ be the position vector of nucleus of the target with respect to Z_P. The momentum transfer $\vec{\alpha}$ in Eq. (2) has the components parallel and perpendicular to $\hat{\vec{v}}$:

$$\vec{\alpha} = \vec{\eta} - \left(\frac{v}{2} - \frac{\Delta E}{v}\right)\hat{\vec{v}}\,, \tag{4}$$

where $\Delta E = E_i - E_f$ with E_i being the binding energy of two-electron target and $E_f = -Z_P^2/(2n^2) - 2$. The transverse component of the change in the relative linear momentum of a heavy particle