

Hydrogen-Impact Ionization Cross Sections in the Bates-Griffing Formalism

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Abstract

We describe a simple and effective procedure to estimate the hydrogen-impact ionization cross sections over an energy range relevant to studies of ACR heliospheric transport. The procedure is valid in the first Born approximation using known or estimated electron-impact cross sections. The original Bates-Griffing relation between the two sets of cross sections is reexpressed and a correction factor due to multiple transitions is introduced. Sample cross sections calculations for He, C, O and Ne collisions with hydrogen are presented.

1 Introduction:

Hydrogen-impact ionization cross sections for light ions in the energy range of \sim keV/nucleon to few hundreds of MeV/nucleon are poorly known for many reactions of interest to astrophysics and plasma physics. The corresponding ionization rates are needed in models of the heliospheric transport of multiply-charged ACR (e.g., Jokipii 1996) as well as in high-temperature plasma confinement studies. In particular, for ACR studies these rates can affect (essentially via coupling) significantly the acceleration, transport, as well as the charge distribution of the ACR ion species.

For the energy range of interest to ACR studies, the first Born approximation can be used to estimate the cross section σ_p for the ion-hydrogen electron-loss process (e.g., McDowell & Coleman 1970)



if the ion's kinetic energy is above a certain threshold energy E_B , which is ionization-potential dependent. In process (1), H^* denotes all bound and continuum states of H, but without specifying the states, while e' denotes the ejected electron, which can emerge with some kinetic energy imparted to it. The same approximation can also be applied for σ_e from the electron-impact process



The original Bates-Griffing relation (Bates & Griffing 1953) is a general, but open, functional between the two sets of cross sections for the above two processes. For the same incident relative velocity and at high enough energies (i.e., the incident kinetic energy $\gg E_B$), the two cross sections approach a single value. For energies below this asymptotic region, which are more relevant to ACR transport studies, the Bates-Griffing relation gives σ_e in terms of σ_p as a functional since the incident kinetic energies do not directly correspond to each other. The functional is not closed in the sense that σ_p is evaluated at two different energy points in order to estimate σ_e at a single energy point that corresponds to the same incident velocity.

The availability of E_B -dependent, parametric estimates for σ_e (e.g., Arnaud & Rothenflug 1985; Shevelko et al. 1983) makes estimating σ_p using a relation like the Bates-Griffing possible. To that end, we will express σ_p as a closed functional of σ_e using the Bates-Griffing relation in the first Born approximation. In addition, a correction factor associated with multiple transitions, i.e., sum over shells, is introduced. The procedure is only meant to give a crude, but robust, first-order approximation to needed cross sections that otherwise either have not been measured or are difficult to calculate theoretically. Sample applications to the direct-impact ionization of He, C, O and Ne in collisions with hydrogen, a set of particular relevance to ACR, are presented, along with some available data for He and C.

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2 The Bates-Griffing Relation:

In the first Born approximation the collision is approximated as a transition from continuum-to-continuum states. In the center-of-mass frame the initial and final wavefunctions become pure momentum states of a single particle, and the transition matrix is essentially determined by a Coulombic potential and the amount of momentum transfer in the collision. For processes (1) and (2), ignoring any energy imparted to the ejected electron, the Born cross section is written as

$$\sigma_B(E_e) = \frac{8}{\pi E_e} \int_{k_{\min}}^{k_{\max}} dk k^{-3} |\mathcal{M}_{fi}|^2, \quad (3)$$

where E_e is the electron's incident kinetic energy, $k = k_i - k_f$ is the relative momentum, and k_i and k_f are the initial and final relative momenta. The limits k_{\min} and k_{\max} are determined from energy conservation, and are dependent on the incident particle. Kinematically, the two cross sections σ_e and σ_p are different because these limits are different. For a single transition with ionization potential V_j , for protons² the formal limits (Peach 1965) are

$$k_{\min} = \frac{V_j}{2k_i} \left(1 + \frac{1}{4} \frac{m_e V_j}{\mu E_e} \right); \quad k_{\max} \rightarrow \infty, \quad (4)$$

where m_e is the electron's rest mass and μ the reduced mass of the ion-hydrogen system. For electrons the limits become

$$k_{\min} = k_i - k_i \left(1 - \frac{V_j}{E_e} \right)^{1/2}; \quad k_{\max} = k_i + k_i \left(1 + \frac{V_j}{E_e} \right)^{1/2}. \quad (5)$$

The matrix elements \mathcal{M}_{fi} need not be evaluated explicitly. Instead, Eq. (3) for protons can be written as

$$\sigma_p(E_p; k) = \frac{\mu}{m_e} \frac{\mathcal{W}(k)}{E_p}, \quad (6)$$

where E_p is the proton's incident kinetic energy such that k_{\min} is the same in both the ion-electron and ion-proton systems. The function \mathcal{W} , whose exact form is not required, is defined as

$$\frac{d\mathcal{W}(k)}{dk} \propto -k^{-3} |\mathcal{M}_{fi}|^2, \quad (7)$$

with the property that in the limit $k \rightarrow \infty$, $\mathcal{W} \rightarrow 0$. Similarly, for electrons the Born cross section becomes

$$\sigma_e(E_e; k) = \frac{\mathcal{W}(k) - \mathcal{W}(k')}{E_e}, \quad (8)$$

where $k' = V_j/k$.

Now, realizing that $E_e(k) = (\gamma m_e / \mu) E_p(k)$, with $\gamma = (1 + E_B / E_p)^2$ and $E_B = \mu V_j / (4m_e)$, the Bates-Griffing relation for σ_e in terms of σ_p is written as

$$\sigma_e(E_e; k) = \gamma^{-1} \left[\sigma_p(E_p; k) - \frac{E_p'}{E_p} \sigma_p(E_p'; k') \right] \quad (9)$$

with $E_p' = E_B^2 / E_p$. Note that in Eq. (9) σ_p needs to be evaluated at two different energy points, E_p and E_p' , corresponding to two different relative momenta, k and k' , in order to estimate σ_e at the energy point E_e . As such the Bates-Griffing relation for σ_e in terms of σ_p is not a closed one. Next, we show how one can, to first order in $(k - k')$, reexpress the Bates-Griffing relation for σ_p in terms of σ_e at the same k .

²We treat atomic hydrogen as a proton because the correction factor (in \mathcal{M}_{fi}) due to the bound electron behaves like k^{-4} in Eq. (3), which is negligible for the energy range of interest here.

3 Expressing σ_p in terms of σ_e :

To express σ_p as a closed functional of σ_e , Taylor expand $\sigma_p(E_p; k)$ about $\sigma_p(E'_p; k')$ to first order in $(k - k')$ as

$$\sigma_p(E_p; k) = \sigma_p(E'_p; k') + (k - k') \frac{d\sigma_p(E_p; k)}{dk}. \quad (10)$$

From Eqs. (6) and (8), to first order in $(k - k')$ with $\mu' = \mu/m_e$, we have

$$\frac{d\sigma_p(E_p; k)}{dk} = \frac{\mu'}{E_p} \frac{d\mathcal{W}}{dk} + \mu' \mathcal{W} \frac{dE_p^{-1}}{dk}, \quad (11)$$

$$\frac{d\mathcal{W}}{dk} = \frac{\mathcal{W}(k) - \mathcal{W}(k')}{k - k'} = \frac{E_e}{k - k'} \sigma_e(E_e; k). \quad (12)$$

Upon substituting Eqs. (11) and (12) in Eq. (10) and equating terms with Eq. (9), we get

$$\sigma_p(E'_p; k') = -\frac{k - k'}{1 - \epsilon^2} \mu' \mathcal{W} \frac{dE_p^{-1}}{dk} = \frac{2}{1 + \epsilon} \sigma_p(E_p; k), \quad (13)$$

where $\epsilon = E_B/E_p$ and $E_p = 1/4\mu'k^2$. Eliminating $\sigma_p(E'_p; k')$ in Eq. (9) and solving for $\sigma_p(E_p; k)$ gives

$$\sigma_p(E_p; k) = \gamma \left(1 - \frac{2\epsilon^2}{1 + \epsilon}\right)^{-1} \sigma_e(E_e; k), \quad (14)$$

which is a closed relation for σ_p in terms of σ_e at the same k .

Finally, since the Arnaud & Rothenflug (1985) estimates we use for σ_e are shell dependent and the above relation for σ_p depends on each shell parametrically, the total, i.e., sum over shells, cross section becomes

$$\sigma_p(E_p; k) = \frac{1}{2}(1 + N^2) \sum_{j=1}^N \sigma_p^j(E_p; k)/j^2, \quad (15)$$

where N is the number of shells and $\sigma_p^j(E_p; k)$ is given by Eq. (14) for each ionization potential V_j . The factor $1/2j^2$ assumes hydrogen-like degeneracy and $(1 + N^2)$ is a normalization factor.

To illustrate, in Fig. 1 we show calculated ionization cross sections for helium and carbon where some available data are also shown. Fig. 2 shows similar cross sections for oxygen and neon. An implementation of this formalism in F77/90, C, or C++ portable routines along with the shells' parameters data files (for He, C, O, N, and Ne) are available upon request from the author. Implementation for other elements where estimates (or data) for σ_e are available is straightforward.

Work has been supported by NSF grant no. 9810653 and NASA-JOVE grant no. NAG8-1208.

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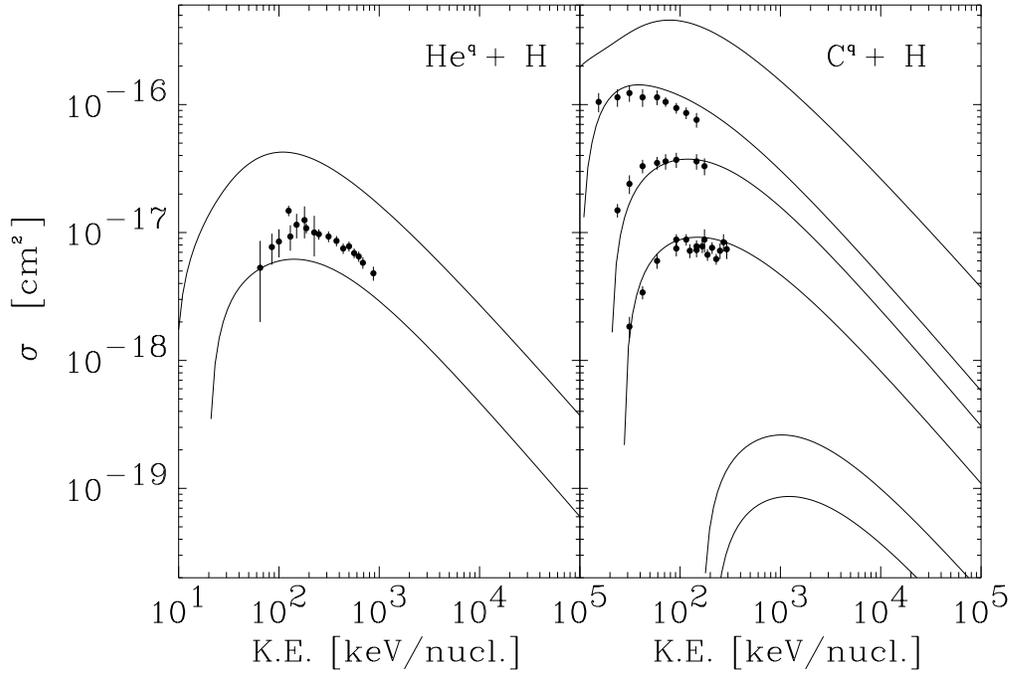


Figure 1: Hydrogen-impact ionization cross sections for He and C. Data for He are from Watts et al., Peart et al., and Sant'Anna et al., and from Goffe et al. and Sant'Anna et al. for C.

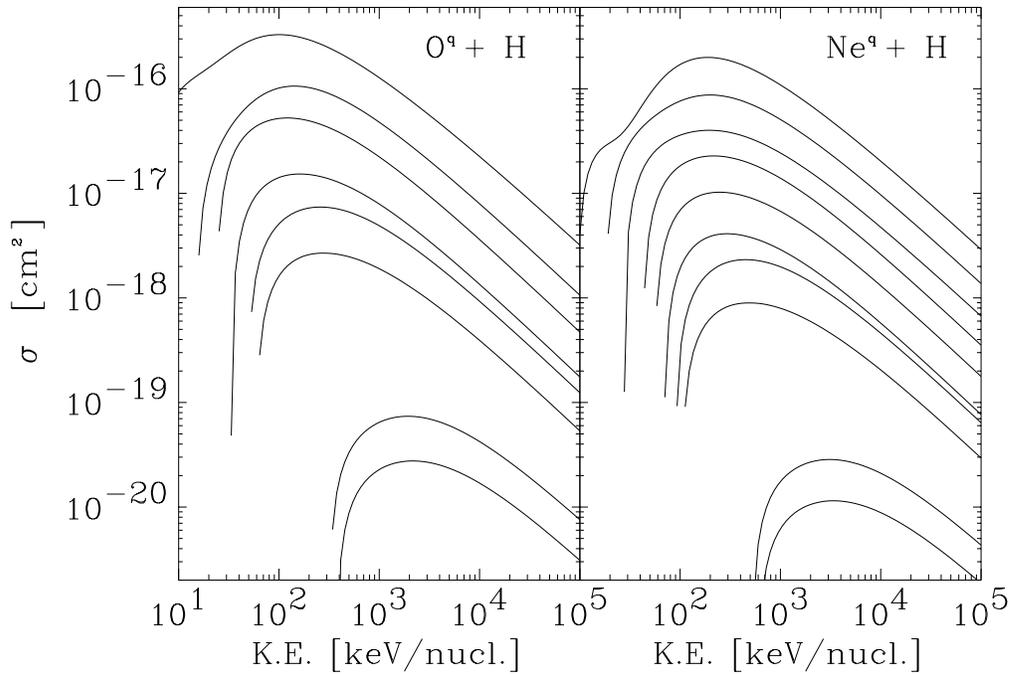


Figure 2: Hydrogen-impact ionization cross sections for O and Ne. In both figures, curves depict the cross sections $\sigma_{0 \rightarrow 1}, \sigma_{1 \rightarrow 2}$, etc., and terminate as the kinetic energy $E_p \rightarrow E_B^+$.