Charge-exchange source terms in magnetohydrodynamical plasmas

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Abstract. In the modeling of space plasma environments, source terms are often used to couple separate species of particles and/or fluids. There have been many techniques developed over the years to make such coupling more tractable while maintaining maximum physical fidelity. In our current application we use the formalism of the Boltzmann collision integral to compute source terms due to charge-exchange events in the heliosphere. The charge-exchange cross sections often encountered in heliospheric interactions can be fit to laboratory data, but in most cases cannot be directly integrated over analytically. Therefore, researchers often employ various levels of approximation, either semi-analytic or numerical. We explore several assumptions to the charge-exchange source term integrals, namely using Maxwellian velocity spaces for like-mass species and either hard-sphere, power-law, or exact forms of the cross section.

1. Introduction
Modeling of the interaction between the solar wind (SW) and local interstellar medium (LISM) dates back to the dawn of the space age, [1–4]. As knowledge of properties of the SW and LISM improved, the models correspondingly began to include more sophisticated physics. The LISM is a partially ionized gas [5] where LISM hydrogen ions and neutrals are weakly coupled by photoionization and charge-exchange [6, 7]. The crossing of the termination shock in 2004 and 2007 by NASA’s Voyager 1 & 2 spacecraft [8, 9], respectively, and the transition into interstellar space by Voyager 1 in 2012 [10] have provided invaluable data to the heliospheric modeling community. In addition, the Interstellar Boundary Explorer (IBEX) [11], launched in October 2008, has been making observations of energetic neutral atoms (ENAs), which discovered the IBEX ribbon and has shed light on the structure of the heliosphere, interstellar matter, and several other scientific areas (see [12] for a complete list of discoveries). The accepted theory of the generation of the IBEX ribbon is the secondary ENA mechanism [13, 14], which includes charge-exchange in the micro physics between the LISM plasma and ENAs.

It was shown qualitatively by Wallis [7] that resonant charge-exchange between hydrogen atoms and protons greatly influences the structure and location of the termination shock and heliopause. Since that time it has commonly been accepted that this charge-exchange mechanism is a critical ingredient for models of the heliosphere. Other collision mechanisms, both inelastic and elastic, may also contribute in modifying the global structure of the heliosphere. As pointed out by Williams et al. [15], momentum exchange for H-H and H-p collisions are equally as frequent as charge-exchange, with mean free paths of ~200 AU outside the heliosphere. This may degrade the distinction between the separate populations of hydrogen atoms (interstellar, ENA,
etc.) and act to thermalize them to a common temperature. In this paper we will solely focus on resonant charge-exchange with same-mass, Maxwellian distributed velocity space species.

Two popular simulation methods used to model the heliosphere are the fluid/multi-fluid and fluid-kinetic simulations, where the fluids are either hydrodynamic (HD), magnetohydrodynamic (MHD), or both. The ions are always HD/MHD fluids, while the neutrals may be a single fluid, ensemble of fluids, or kinetic particles. The self consistent problem of the SW-LISM interaction, including resonant charge-exchange, was considered by [16, 17] using a fluid approach, see also [18–21]. Examples of a multi-fluid approach include [15, 22, 23]. The work of Malama [24] introduced the kinetic treatment of neutral hydrogen via the Monte Carlo method, leading to the paper of Baranov & Malama [25] solving the problem using charge-exchange source terms to couple particle neutrals to a fluid plasma. However, the effects of the interplanetary and interstellar magnetic fields were ignored. A decade or so later, the modeling groups of [26–28] adopted the Monte Carlo kinetic approach along with a MHD description of the proton/electron mixture. For the sake of brevity, in this paper we will limit discussion to source terms that couple the fluid ions and fluid neutrals via resonant charge-exchange.

In the past, authors have only compared the analytic solutions of the hard-sphere or power-law source term approximations to their asymptotic forms (e.g., [19, 29, 30]). However, comparisons to numerical evaluations of the exact source term integrals have not been done thus far, and are necessary in determining the effectiveness of these different approximations for various parameter domains. The purpose of this paper will be to analyze the relative errors of these approximations to the exact source term integrals for a range of effective temperatures as well as specific cases of parameters particular to the heliosphere.

In §2 we will outline the results of using two Maxwellian fluids (one ion and one neutral) in the collision source term integrals while keeping the form of the charge-exchange cross section generalized. Then, in §3 we will proceed to derive expressions for power-law and in §4 for hard-sphere (constant over integral) cross sections, as a special case of the power-law formalism. Proceeding to §5.1 we will compare the numerical results of using the exact, power-law, and hard-sphere forms of the charge-exchange cross section for the momentum and thermal energy source terms for a range of effective temperatures. §5.2 will be dedicated to specific cases of temperatures and bulk velocities for protons and hydrogen atoms in the heliosphere. Finally, we will summarize in §6.

2. Resonant charge-exchange source terms

To begin, we will assume elastic, resonant, charge-exchange collisions between protons and hydrogen atoms. The following calculations will be done for the mass, momentum, and energy sources imparted on the proton population, but analogous equations can be found for the hydrogen population by swapping the p and H subscripts. Under the theory of the Boltzmann collision integral for isotropic cross sections we can write (e.g., [31]),

\[
\begin{align*}
\{ Q_n, Q_M, Q_{Etot} \} &= \int \int d^3v_p d^3v_H |v_H - v_p| \sigma_{ex}(|v_H - v_p|) f_p f_H \Delta \xi_{Hp},
\end{align*}
\]

where the source term moments are,

\[
\Delta \xi_{Hp} = \begin{cases} 
m_H - m_p \approx 0 & \text{mass} \\
m_H v_H - m_p v_p = m(v_H - v_p) & \text{momentum} \\
\frac{1}{2}m_H v_H^2 - \frac{1}{2}m_p v_p^2 = \frac{1}{2}m(v_H^2 - v_p^2) & \text{total energy}
\end{cases}
\]

and \( \sigma_{ex} \) is the charge-exchange cross section (e.g., [32] or [33]). The mass density source equates to zero because the p-H charge-exchange reaction is symmetric. Throughout this paper we will
assume that the proton and hydrogen masses are the same, viz. \( m \equiv m_H = m_p \). The p-H charge-exchange cross section is parametrized in [32] by the following expression,

\[
\sigma_{ex}(E) = (a_1 - a_2 \ln E)^2 \left(1 - e^{-a_3/E}\right)^{4.5} \quad \text{for } E \in [0.005, 250] \text{ keV},
\]

(3)

where \( a_1 = 4.15, a_2 = 0.531, a_3 = 67.3 \text{ keV}, \) and \( E \) in units of keV with \( \sigma_{ex} \) in units of \( 10^{-16} \text{ cm}^2 \). The distribution functions of the protons and hydrogen atoms, \( f_p \) and \( f_H \), are assumed to be Maxwellian (i.e., independently in local thermal equilibrium) such that,

\[
f_p f_H = \frac{n_p n_H}{\pi^3 v_{tp}^2 v_{tH}^2} \exp \left[-\frac{(v_p - u_p)^2}{v_{tp}^2} - \frac{(v_H - u_H)^2}{v_{tH}^2}\right],
\]

(4)

where \( n_p \) & \( n_H \) are the number densities, \( u_p \) & \( u_H \) the bulk flow velocities, and \( v_{tp} \) & \( v_{tH} \) the thermal speeds defined by the temperature as \( v_i = \sqrt{2k_B T_i/m_i} \) for each species, \( k_B \) is the Boltzmann constant and \( T_i \) and \( m_i \) are the temperatures and masses of the species. The macroscopic variables \( n_i, u_i, \) and \( T_i \) are implied to be functions of position and time, independent of the phase space variables \( v_i \), for \( i = p,H \). Next, we define the center of mass velocity \( V \) and relative velocity \( g \) (see e.g., [29, 31]) such that

\[
V = \frac{m_p v_p + m_H v_H}{m_p + m_H} \approx \frac{1}{2}(v_p + v_H)
\]

(5)

\[
g = v_H - v_p
\]

(6)

or writing the original velocities in terms of the new definitions,

\[
v_H = V + \frac{1}{2}g
\]

(7)

\[
v_p = V - \frac{1}{2}g
\]

(8)

Note that the Jacobian of this transformation is equal to 1. To proceed with evaluating Eq. (1) we first integrate over the center of mass velocity. The following definitions aid with simplifying the notation:

\[
\Delta u = u_H - u_p
\]

(9)

\[
U = \frac{u_p v_{tH}^2 + u_H v_{tp}^2}{v_t^2}
\]

(10)

\[
\Delta v_t^2 = v_{tH}^2 - v_{tp}^2
\]

(11)

\[
v_t^2 = v_{tH}^2 + v_{tp}^2.
\]

(12)

After the change of variables of Eqs. (5) and (6), the exponent of Eq. (4) reads

\[
-\frac{v_t^2}{(v_{tp}v_{tH})^2} \left[V^2 + V \cdot X + b\right]
\]

(13)

where

\[
X = -\frac{\Delta v_t^2}{v_t^2}g - 2U
\]

(14)

\[
b = \frac{1}{4}g^2 + g \cdot U + \frac{u_p^2 v_{tH}^2 + u_H^2 v_{tp}^2}{v_t^2}.
\]

(15)
We choose $\mathbf{X}$ to be aligned along the $z$-axis and the perpendicular component of $\mathbf{g}$, with respect to $\mathbf{X}$, along the $\mathbf{x}$-axis in a spherical coordinate system. This choice makes the integration over the azimuthal angle $\phi$ trivial, as well as for the polar angle $\cos \theta = \mu$, where $\hat{\mathbf{v}} \cdot \hat{\mathbf{X}} = \mu$. The integral over $\mathbf{g}$ is done in a similar manner; we integrate via a spherical coordinate system with the $z$-axis aligned along $\Delta \mathbf{u}$, simplifying the azimuthal integration.

Since the charge-exchange cross section is only a function of the magnitude of $\mathbf{g}$ we can compute all but the last integral over $g$. We then arrive at

$$Q_M = \frac{2mn_p n_H}{\Gamma(3/2) v_i^3} \int_0^\infty dg \sigma_{ex}(g) g^4 e^{-\frac{g^2 + \Delta u^2}{v_i^2}} i_1 \left( \frac{2g \Delta u}{v_i} \right) \Delta \hat{u}$$

(16)

$$Q_{E_{tot}} = Q_M \cdot U + \frac{mn_p n_H \Delta v_i^2}{\Gamma(3/2) v_i^2} \int_0^\infty dg \sigma_{ex}(g) g^5 e^{-\frac{g^2 + \Delta u^2}{v_i^2}} i_0 \left( \frac{2g \Delta u}{v_i^2} \right)$$

(17)

where $\Gamma$ is the gamma function and $i_n$ is the modified spherical Bessel function of the first kind, for the momentum and total energy charge-exchange source terms, in agreement with Eqs. (25) and (27) of McNutt et al.’s work [29]. Notice that the first and second term of $Q_{E_{tot}}$ represents the kinetic and thermal energy source denoted by $Q_{E_K}$ and $Q_{E_T}$, respectively.

From Eq. (17) we can understand the physical meaning of $\mathbf{U}$, namely, the kinetic energy source is given by the component of the momentum source in the direction of $\mathbf{U}$. There is a bias towards the bulk flow of the cooler species for the direction of $\mathbf{U}$. In this sense, the hotter species has less of an effect on the overall kinetic energy source, albeit a greater influence on the thermal energy source.

### 3. Power-law cross section approximation of source terms

Given cross sections that vary slowly with the collision energy (i.e., relative speed $g$), we can model the cross section as having a power-law form given by,

$$\sigma_{ex}(g) \sim \sigma_0 \left( \frac{g}{g_0} \right)^\nu$$

(18)

similar to Eq. (1) of [30], where $g_0$ is the effective relative speed, $\sigma_0 = \sigma_{ex}(g_0)$ the cross section, and $\nu$ the power-law index. Inserting Eq. (18) into Eqs. (16)-(17) and using the substitution $z = g^2 \Delta u^2 / v_i^2$, we arrive at the intermediate step,

$$Q_M = \frac{mn_p n_H \sigma_0}{\Gamma(3/2) v_i^2 g_0^2} \left( \frac{v_i^2}{\Delta u} \right)^{2\nu+5} e^{-\frac{\Delta u^2}{v_i^2}} \int_0^\infty dz \frac{z^{\nu+3/2}}{\sqrt{\pi}} \frac{e^{-z}}{v_i^2} i_1(2\sqrt{z}) \Delta \hat{u}$$

(19)

$$Q_{E_{tot}} = Q_M \cdot U + \frac{mn_p n_H \sigma_0 \Delta v_i^2}{\Gamma(3/2) v_i^2 g_0^2} \left( \frac{v_i^2}{\Delta u} \right)^{2\nu+5} e^{-\frac{\Delta u^2}{v_i^2}} \int_0^\infty dz \frac{z^{\nu+2}}{\sqrt{\pi}} \frac{e^{-z}}{v_i^2} i_0(2\sqrt{z})$$

(20)

To proceed we use the following confluent hypergeometric function substitutions, which can be derived by matching the power series of the confluent hypergeometric and hyperbolic functions

$$\, _0F_1(-; 3/2; t) = \frac{\sinh(2\sqrt{t})}{2\sqrt{t}} = i_0(2\sqrt{t})$$

(21)

$$\, _0F_1(-; 5/2; t) = \frac{3}{4t} \left[ \cosh(2\sqrt{t}) - \frac{\sinh(2\sqrt{t})}{2\sqrt{t}} \right] = \frac{\Gamma(5/2)}{\Gamma(3/2)\sqrt{t}} i_1(2\sqrt{t})$$

(22)
the integral
\[ \int_0^\infty t^{\alpha-1} \exp(-at)F_1(-b; t)dt = a^{-\alpha} \Gamma(\alpha)F_1(\alpha; b; 1/a), \quad (23) \]
derived from the general form in Eq. 7.522.5 of Gradshteyn & Ryzhik [34], and Kummer’s transformation, Eq. 13.1.27 of Abramowitz & Stegun [35],
\[ e^{-t}F_1(a; b; t) = F_1(b-a; b; -t). \quad (24) \]

Applying these substitutions and transformation we obtain,
\[ Q_M = A_\nu \Delta u G_{1,\nu} \left( \frac{\Delta u}{v_t} \right) \]
\[ Q_{E_{tot}} = Q_{E_K} + Q_{E_T} = Q_M \cdot U + \frac{1}{2} A_\nu \Delta v_t^2 G_{2,\nu} \left( \frac{\Delta u}{v_t} \right), \quad (26) \]
where the coefficient \( A_\nu \) and functions \( G_{1,\nu}(x) \) and \( G_{2,\nu}(x) \) are,
\[ A_\nu = \frac{m n \eta H \sigma_0 v_t}{(g_0/v_t)^{2\nu}} \]
\[ G_{1,\nu}(x) = \frac{\Gamma(\nu+3)}{\Gamma(5/2)} F_1 \left[ -\nu - \frac{1}{2}, \frac{5}{2}; -x^2 \right], \quad (28) \]
\[ G_{2,\nu}(x) = \frac{\Gamma(\nu+3)}{\Gamma(3/2)} F_1 \left[ -\nu - \frac{3}{2}, \frac{3}{2}; -x^2 \right], \quad (29) \]
and \( F_1 \) the Kummer confluent hypergeometric function. Note we recover Eq. (23) of [30].

It can be observed that if both the proton and hydrogen species have the same bulk velocity there will be no net exchange in momentum. However, for different temperatures there will be exchange in energy transferred from the hotter species to the colder species. On the other hand, if the species have the same temperature but different bulk flow velocities, the sign of the momentum and energy exchange is determined by the sign of \( \Delta u \). Finally, if both the bulk flows and temperatures are the same, the species are in equilibrium with each other and there is no net exchange of momentum or energy, even though charge-exchange events will occur.

In numerical applications, it is beneficial to use simplified forms of Eqs. (25)-(26) by matching the first order term of the Taylor and asymptotic series for small and large values of \( x = \Delta u/v_t \) to a model function,
\[ \left[ a x^2 + b^{1/(\nu+\frac{3}{2})} \right]^{\nu+\frac{3}{2}}. \quad (30) \]
By doing so, and factoring the coefficients such that \( a = 1 \), it can be shown that,
\[ G_{1,\nu}(x) \approx \left[ x^2 + \left( \frac{\Gamma(\nu+3)}{\Gamma(5/2)} \right)^{1/(\nu+\frac{3}{2})} \right]^{\nu+\frac{3}{2}}, \quad (31) \]
\[ G_{2,\nu}(x) \approx \left[ x^2 + \left( \frac{\Gamma(\nu+3)}{\Gamma(3/2)} \right)^{1/(\nu+\frac{3}{2})} \right]^{\nu+\frac{3}{2}}, \quad (32) \]
where Eq. (31) is analogous to Eq. (31) of [30]. Therefore, Eqs. (31)-(32) are said to be asymptotic to Eqs. (28)-(29) for \( x \ll 1 \) or \( x \gg 1 \). From a practical standpoint, using a single constant for the power-law index \( \nu \) fails for most regimes of the p-H cross section, even when
using a clever effective relative speed $\bar{v}$, e.g., [30]. To combat this issue, it is useful to adopt a variable power-law given by,

$$\nu = \frac{1 \text{ keV}}{2\Delta E} \ln \left[ \frac{\sigma_{\text{ex}}(E_0 e^{\Delta E/1 \text{keV}})}{\sigma_{\text{ex}}(E_0 e^{-\Delta E/1 \text{keV}})} \right].$$

Eq. (33) is derived (see Appendix) from the central difference method by taking the Taylor expansion of the logarithm of the cross section with respect to the logarithm of the collision energy $E_0 = \frac{1}{2} m (\Delta u)^2$. The energies $\Delta E$ and $E_0$ are in units of keV, and $\Delta E$ is some small change in energy, typically $< 0.001$ keV for our purposes. The cross section in $A_\nu$ should then be evaluated at $\Delta u$ and not $\bar{v}$. As an illustration, Figure 1 is an application of Eq. (33) using $\sigma_{\text{ex}}$ of Eq. (3).

![Diagram showing a power-law index fit to the p-H charge-exchange cross section](image)

Figure 1: A power-law index fit to the p-H charge-exchange cross section [32] using Eq. (33). The exponential cutoff becomes noticeable for energies greater than $\sim 10$ KeV.

### 3.1. Physical interpretation of power-law cross section

An interesting consequence of using a power-law cross section, as defined in Eq. (18), is that the charge-exchange cross section can be thought of as the result of scattering by repulsion of a central force, given by $F = K_{ab} r^{-p}$, where $K_{ab}$ is some constant that depends on the physical application (see Eq. 9.15 of [31] and pg. 172 of [36] for specific examples) and $r$ is the distance between particles $a$ and $b$. A typical central force found in nature is the Coulomb interaction, were $p = 2$ and $K_{ab} = q_a q_b / (4\pi\epsilon_0)$, where $q_i$ are the charges of each species and $\epsilon_0$ is the permittivity of free space.

From the Appendix of Section 9 of [31] we see that $\nu = -2/(p - 1)$ relates the power-law index $\nu$ of the cross section to the central force power index $p$. Common central force laws are Coulomb interactions ($p = 2$, $\nu = -2$), Maxwell molecules ($p = 5$, $\nu = -1/2$), and hard-sphere interactions ($p \to \infty$, $\nu = 0$). The p-H charge-exchange cross section in Eq. (3) has a relatively hard power-law fit in the ranges of 5 eV ($p = 14$, $\nu = -0.154$) to 10 keV ($p = 6$, $\nu = -0.4$) reaching steeper than Coulomb-like interactions for 250 keV ($p = 1.42$, $\nu = -4.76$). See Figure 1 for the full range of energies within the domain of the parameterized fit of Eq. (3).
4. Hard-sphere cross section approximation of source terms

For the hard-sphere approximation, we take \( \nu = 0 \) in Eqs. (25)-(26), and simplify to obtain

\[
G_{1,0}(x) = \frac{8}{3\sqrt{\pi}} F_1 \left[ \begin{array}{c} \frac{1}{2} + \frac{5}{2} + x^2 \\ \frac{1}{2} - 1 \end{array} \right] = \frac{\exp(-x^2/\sqrt{\pi})}{\sqrt{\pi}} \left( 1 + \frac{1}{2x^2} \right) + \text{erf}(x) \left( x + \frac{1}{x} - \frac{1}{4x^3} \right) \\
G_{2,0}(x) = \frac{4}{\sqrt{\pi}} F_1 \left[ \begin{array}{c} \frac{3}{2} + \frac{3}{2} + x^2 \\ \frac{3}{2} - 1 \end{array} \right] = \frac{\exp(-x^2/\sqrt{\pi})}{\sqrt{\pi}} \left( x^2 + \frac{5}{2} \right) + \text{erf}(x) \left( x^3 + 3x + \frac{3}{4x^2} \right),
\]

where \( \text{erf} \) is the error function, comparable to Eqs. (49)-(50) of [29]. See also [6] and [19]. The momentum and total energy charge-exchange source terms for a constant, hard-sphere cross section are then

\[
Q_M = A_0 \Delta u G_{1,0} \left( \frac{\Delta u}{v_t} \right) \\
Q_{E_{tot}} = Q_{E_K} + Q_{E_T} = Q_M + \frac{1}{2} A_0 \Delta v_t^2 G_{2,0} \left( \frac{\Delta u}{v_t} \right),
\]

where \( A_0 = mn_p n_H \sigma_0 |v| \) and \( \sigma_0 = \sigma_0(\bar{v}) \), to be evaluated at the effective relative speed \( \bar{v} \). The definition of \( \bar{v} \) is not unique, so we will take some time to discuss some variations of this definition in §4.1. We may also simplify \( G_{1,0} \) and \( G_{2,0} \) by plugging \( \nu = 0 \) into Eqs. (31)-(32), obtaining

\[
G_{1,0}(x) \approx \sqrt{x^2 + \frac{64}{9\pi}} \\
G_{2,0}(x) \approx \left[ x^2 + \left( \frac{16}{\pi} \right)^{1/3} \right]^{3/2},
\]

which are asymptotic to Eqs. (34) and (35) for \( x \ll 1 \) or \( x \gg 1 \).

4.1. Effective relative speed

In the case of hard-sphere collisions, the cross section is constant, and can thus be taken outside of the integral during evaluation. In this case it must then be computed at an effective relative speed, \( \bar{v} \). One simple way to define \( \bar{v} \) is via the average interaction rate (e.g., [19, 36]),

\[
\bar{v} = \frac{1}{n_p n_H} \int d^3 v_p d^3 v_H |v_H - v_p| f_p f_H
\]

and for Maxwellian velocity distributions for both species it can be shown that,

\[
\bar{v} = v_t G_{0,0}(x) \\
G_{0,0}(x) = \left[ \frac{\exp(-x^2/\sqrt{\pi})}{\sqrt{\pi}} + \left( \frac{1}{2x} + x \right) \text{erf}(x) \right] \approx \sqrt{\frac{4}{\pi}} + x^2
\]

where \( x = \Delta u/v_t, \Delta u = |u_H - u_p| \), and \( v_t^2 = v_{tH}^2 + v_{tP}^2 \). This definition of \( \bar{v} \) is used for the effective relative speed for the number, momentum, and total energy source in [19], in contrast to the next definition (see Eqs. (44)-(46)).

For the hard-sphere approximation the cross section is Taylor expanded, as explained by [29], around an effective relative speed \( g_0 \),

\[
\sigma_{ex}(g) = \sigma_0 + \left( \frac{d \sigma_{ex}}{dg} \right)_{g=g_0} (g - g_0) + \cdots
\]
where $g_0$ is found such that the integral over the second term vanishes, for each moment $1$, $g$, and $g^2$, thereby eliminating first order errors. We assume that higher than first order terms are insignificant compared to lower order terms of the Taylor series expansion. Therefore, omitting the details (see Appendix B of [37] for a similar discussion) we find that the effective relative speeds for the number, momentum, and total energy sources are, using $x = \Delta u/v_t$

$$
\bar{v} = \frac{3\sqrt{\pi}}{4} v_t \frac{1}{1F_1} \left[-1; \frac{3}{2}; -x^2\right] = v_t \frac{x^2 + \frac{3}{2}}{G_{0,0}(x)} \approx v_t \sqrt{x^2 + \frac{9\pi}{16}} \quad (44)
$$

$$
\bar{v}_m = \frac{15\sqrt{\pi}}{16} v_t \frac{1}{1F_1} \left[-1; \frac{5}{2}; -x^2\right] = v_t \frac{x^2 + \frac{5}{2}}{G_{1,0}(x)} \approx v_t \sqrt{x^2 + \frac{225\pi}{256}} \quad (45)
$$

$$
\bar{v}_E = \frac{15\sqrt{\pi}}{16} v_t \frac{1}{1F_1} \left[-\frac{3}{2}; \frac{3}{2}; -x^2\right] = v_t \frac{x^4 + 5x^2 + \frac{15}{4}}{G_{2,0}(x)} \approx v_t \sqrt{x^2 + \frac{225\pi}{256}}. \quad (46)
$$

The right hand sides of both Eqs. (45) and (46) are the same due to the fact that in the analytic equations, the leading order term of the Taylor series at $x = 0$ are identical. The asymptotic forms of Eqs. (42) and (44)-(46) are valid for $x \ll 1$ or $x \gg 1$, i.e., when $\Delta u < v_t$ or $\Delta u > v_t$.

5. Comparison of the exact, power-law, and hard-sphere cross section in source term integrals

5.1. Range of temperature sums

![Average Relative Error -- Momentum Source](image1)

![Average Relative Error -- Thermal Energy Source](image2)

Figure 2: The average relative error of the momentum source (left) and the thermal energy source (right) of various cross-section approximations found in [19], [29] and this work, as a function of the temperature sum, $T_{sum}$ (see Eq. (47)). The solid curves are analytic expressions while the dotted curves are asymptotic expressions of the hard-sphere and power-law cross section approximations.

In this section we will compare the hard-sphere approximation using the effective relative speeds from either Eqs. (41) or (45)-(46), found in Pauls et al. [19] and McNutt et al. [29], respectively, with the numerical evaluation of the exact momentum and thermal energy source term integrals, given in Eq. (16) and the second term $Q_{ET}$ of Eq. (17). A similar comparison is made for the power-law cross section using a variable power-law index (defined in Eq. (33)) that is fit to the exact cross section in Eq. (3). These comparisons are summarized in Table 1.
Table 1: A list of equations used for each approximation of the charge-exchange cross section.

| Approximation | Reference | Hard-sphere | Hard-sphere | Variable power-law |
|---------------|-----------|-------------|-------------|--------------------|
| Analytic      | Pauls et al. 1995 [19] | Eqs. (34)-(35), (41)a | Eqs. (34)-(35), (45)b-(46)b | Eqs. (28)-(29), (33) |
| Asymptotic    | McNutt et al. 1998 [29] | Eqs. (38)-(39), (41)b | Eqs. (38)-(39), (45)c-(46)c | Eqs. (31)-(32), (33) |

The average relative errors for bulk collision energies $E_0 = \frac{1}{2} m (\Delta u)^2$ in the range of $E_0 \in [5 \text{ eV}, 250 \text{ keV}]$ as a function of the temperature sum,

$$T_{sum} = \frac{mv_t^2}{2k_B} = T_H + T_p,$$

are illustrated in Figure 2 for the cases in Table 1. For low collision energies $E_0$ the exponential cut-off of the charge-exchange cross section (see Eq. (3)) does not play a role. However, for larger collision energies the situation changes; the temperature sum acts as a scaling factor for the cross section argument and for sufficiently large temperature sums, $T_{sum} \sim 10^6 \text{ K}$, all approximations begin to suffer due to the non-linear and non-power-law nature of the exact cross section. In other words, the Maxwellian distribution becomes very broad for large thermal speeds and begins to feel the higher order terms of the Taylor series of the cross section such that the constant, linear, or power-law approximations become inadequate. This is especially true near the exponential cut-off in the cross section above $\sim 10 \text{ keV}$ (see Eq. (3)).

Examining Figure 2, the power-law formalism completely fails for large temperature sums $T_{sum} \geq 5 \times 10^7 \text{ K}$, because of the convergence issues resulting from large, negative power-law indices from high collisional energies. Physically, this translates to inverse power-law forces steeper than Coulomb interactions, which would require a finite cutoff of the integral bounds for convergence. For $T_{sum} < 1 \times 10^6 \text{ K}$, the analytic expressions for the hard-sphere, using the effective relative velocity in [29], and variable power-law approximations produce the best accuracy compared with the exact expressions. Because of the computationally expensive hypergeometric functions used in the variable power-law expressions, it is suggested that the manageable forms of the hard-sphere approximation of [29] or the asymptotic variable power-law forms be used alternatively.

If generalized Lorentzian velocity distributions (i.e., kappa distributions) are used instead of Maxwellian distributions, then the power-law and hard-sphere assumptions of the charge-exchange cross section do not necessarily hold. For example, Heerikhuisen et al. [38] showed differences between assuming either Maxwellian or kappa velocity space distributed protons charge-exchanging with hydrogen atoms in the inner heliosheath (IHS). They showed that a constant, hard-sphere assumption of the cross section produces inaccurate charge-exchange rates, even for moderate temperatures, because the wings (i.e., power-law suprathermal protons) of the kappa distribution extend dozens of thermal speeds when $\kappa \leq 2$.

5.2. Specific cases in the heliosphere
In the heliospheric environment there are a wide variety of thermal and flow conditions for the ions and neutral atoms. We outline the parameters used for three test cases found in the supersonic SW, IHS, and outer heliosheath (OHS) in Table 2.

From Table 3 we can see that the most consistent performing approximation across all cases is the analytic form of McNutt et al. [29]. All approximations perform well in Case 1 in the
Table 2: List of temperatures and bulk velocities, evaluated at various locations along the LISM flow vector in the nose direction of the heliosphere, for protons and pickup ions (PUIs) in the SW, IHS, or OHS that may charge-exchange with neutral hydrogen atoms or hydrogen energetic neutral atoms (H ENAs).

| Case                                  | Temperature [K] | Bulk Velocity [km s$^{-1}$] |
|---------------------------------------|-----------------|-----------------------------|
|                                       | $T_p$           | $T_H$                       | $u_p$ | $u_H$ |
| 1. SW protons with LISM H             | $1 \times 10^5$ [39] | $7.5 \times 10^3$ [40]  | +400 [41] | −25 [40] |
| 2. IHS PUIs with LISM H              | $1.6 \times 10^7$ [39] | $7.5 \times 10^3$ [40]  | +78 [42] | −25 [40] |
| 3. OHS PUIs with H ENAs              | $4.22 \times 10^6$ [42] | $2 \times 10^5$ [43]   | −10 [42] | +400 [41] |

Table 3: For each case described in Table 2 (both analytic and asymptotic forms) the percent relative errors are calculated with respect to the numerical evaluation of the exact momentum and total energy sources, which are the upper and lower element respectively. The temperature sum and bulk flow differences specific to each case are tabulated for quick reference.

| Case | Hard-sphere, [19] | Hard-sphere, [29] | Variable power-law | Parameters |
|------|-------------------|-------------------|--------------------|------------|
|      | Q$_{m}$ | Ana. | Asymp. | Ana. | Asymp. | Ana. | Asymp. | $T_{sum}$ [K] | $\Delta u$ [km s$^{-1}$] |
| 1.   | 0.338   | 0.396 | 0.152 | 0.030 | 0.032 | 0.124 | 1.08 $\times 10^5$ | −425 |
|      | 0.574   | 0.121 | 0.150 | 0.244 | 0.032 | 0.124 |                     |         |
| 2.   | 20.5 | 20.4 | 3.66 | 3.53 | 22.7 | 22.8 | 1.60 $\times 10^7$ | −103 |
|      | 20.8 | 20.1 | 3.66 | 3.79 | 22.8 | 22.5 |                     |         |
| 3.   | 9.28 | 9.40 | 2.63 | 0.501 | 1.36 | 2.52 | 4.42 $\times 10^6$ | 410 |
|      | 9.15 | 29.3 | 3.85 | 17.6 | 0.047 | 19.3 |                     |         |

supersonic SW, because the temperatures and bulk velocities result in lower collisional energies (see Figure 2). In the IHS for Case 2, the hard-sphere forms found in Pauls et al. [19], more specifically the effective relative speed expression, and variable power-law expressions, derived in this work, suffer because of the large temperature sums. The effective relative speeds defined by McNutt et al. [29] cancel out the first order errors from the hard-sphere approximation (see §4.1), and therefore are sufficient for IHS PUI temperatures. For Case 3, most of the asymptotic forms fail to match the exact source terms while the analytic power-law equations operate the best, although they are computationally expensive to use due to the hypergeometric functions involved.

6. Summary
In §2 we derived simplified, exact source term expressions for a generalized, isotropic cross section assuming charge-exchange collisions between Maxwellian fluids. We then assumed two approximations of the cross section: power-law in §3, and hard-sphere in §4. By using the
p-H charge-exchange cross section from Eq. (3) we showed that all approximations evaluated in this paper introduce noticeable errors for \( T_{\text{sum}} > 10^6 \) K. Power-law source terms fail to converge for \( T_{\text{sum}} \geq 5 \times 10^7 \) K, because of the steeper than Coulomb-like power-law index \( \nu \). For \( T_{\text{sum}} < 10^6 \) K, the most accurate and simple source term expressions are the analytic hard-sphere forms of McNutt et al. [29]. This is solely due to the fact that the effective relative speeds \( \bar{v} \) are chosen to cancel first order errors introduced by a constant cross section, in contrast to \( \bar{v} \) defined in Pauls et al. [19]. For heliospheric applications of Maxwellian fluid ions and neutrals, the analytic source terms derived in McNutt et al. [29] perform consistently, in accordance with Table 3. Finally, we remark that for non-resonant cross sections (e.g., proton-helium charge-exchange \( p+\text{He} \rightarrow \text{H}+\text{He}^+ \) [33]) the hard-sphere and power-law assumptions would be invalid, and exact source term integrals must be derived for non-symmetric reactions with dissimilar masses.

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Appendix
Derivation of Eq. (33): The power-law index \( \nu \) can be extracted from the cross section \( \sigma_{\text{ex}} \), Eq. (3), as a function of collision energy \( E \) by computing the slope of \( \sigma_{\text{ex}} \) on a log-log scale. We first make the substitutions \( y = \ln(\sigma_{\text{ex}} \times 10^{16} \text{ cm}^{-2}) \) and \( x = \ln(E \times 1 \text{ keV}^{-1}) \) in order to convert to a log-log scale. Then, \( \nu \) may be approximated using the central difference method for the derivative,

\[
\nu = \frac{dy}{dx} \sim \frac{y(x + h) - y(x - h)}{2h} \quad \text{as } h \to 0.
\]  

We take \( h = \Delta E \times 1 \text{ keV}^{-1} \) and exponentiate the arguments of \( y \) (to convert back to a linear scale in energy) so that we arrive at

\[
\nu = \frac{1 \text{ keV}}{2\Delta E} \ln \left[ \frac{\sigma_{\text{ex}}(E e^{\Delta E/1\text{keV}})}{\sigma_{\text{ex}}(E e^{-\Delta E/1\text{keV}})} \right]
\]  

where \( E \) is in units of keV.

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