Kinetic Theory in Self-Similar Variables
for Neutral Atoms in Plasma

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Abstract

The kinetics of neutral atoms in a plasma undergoing charge-exchange, ionization, and recombination is considered. It is shown that if the mean-free path divided by the macroscopic scale length is constant, it is possible to introduce self-similar variables in the Boltzmann equation for the neutral particles. This equation is then solved analytically, and the nonlocal transport of heat and particles is calculated. Since the mean-free path increases with increasing energy, a one-sided, high-energy tail is formed in the neutral distribution function. This tail may contribute significantly to the heat and particle fluxes. When this is the case, the fluid approximation of these quantities breaks down at arbitrarily short mean-free paths.

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I. INTRODUCTION

Neutral atoms are abundant in any sufficiently cool and dense plasma, and play an important role in the tokamak edge plasma, especially in the divertor. In a hydrogen plasma, neutral atoms interact with the ions mainly through charge exchange (CX), ionization, and recombination. The dynamics of the neutrals is often (e.g., in plasma edge codes) described by fluid equations taking these processes into account. Neutral fluid equations can be derived rigorously by a systematic (Chapman-Enskog) expansion in $\gamma \equiv \lambda/L$, the mean-free path of the neutral particles, λ, divided by the macroscopic length scale, L.[1-3] This parameter is, however, not always small in practice. For instance, the tokamak scrape-off layer (SOL) is generally only about a centimeter wide, which is usually comparable to the neutral mean-free path. It is therefore desirable to determine exactly when fluid equations are valid. A kinetic treatment of the neutrals is then necessary, and has been carried out in, e.g., Refs. 4-7, where the one-dimensional neutral kinetic equation was solved by means of the Wiener-Hopf technique or by expansion in singular eigenfunctions. These techniques are elegant, though laborious, but suffer from the shortcoming that they are only able to treat a nearly isothermal plasma; the temperature must not vary significantly over a CX mean-free path, a condition clearly not satisfied in a typical tokamak SOL. In addition, it must be assumed that the CX cross section σ be exactly inversely proportional to the relative velocity v_{rel} of the atom and ion participating the in the CX reaction. This assumption was also made in Ref. 8, where the authors were able to treat the case of strong temperature variation under an additional simplifying assumption when calculating the density.

In the present paper, we solve the neutral kinetic equation in an entirely different way, allowing for strong temperature variation as well as for accurate dependence of σ on v_{rel}, but neglecting the role played by boundary conditions. The solution is possible if the ratio γ

of the mean-free path to the temperature length scale is constant throughout the plasma. As shown in Sec. II, it then becomes possible to introduce self-similar variables which reduce the dimensionality of the equation.[9] If the conventional assumption $\sigma \sim 1/v_{rel}$ is made, it is then relatively easy to find the neutral distribution function analytically. This makes it possible to establish bounds on the applicability of fluid equations. Interestingly, it turns out that the condition $\gamma \ll 1$ alone does not ensure that the fluid approximation is valid; an additional constraint also applies. In other words, the Chapman-Enskog expansion fails in certain cases even for arbitrarily small γ! The reason for this is the formation of a tail in the neutral distribution causing it to depart significantly from a Maxwellian at high energies and leading to strongly increased transport. A similar phenomenon occurs for electron heat transport in sufficiently steep temperature profiles.[9] The shape of the tail is expected to be sensitive to the CX cross section σ. The use of a more exact expression for σ than previously employed is therefore investigated in Sec. III. It is shown that although the full kinetic equation is not amenable to analytic solution in this case, it is still possible to obtain the relative distribution of high-energy neutrals. These particles not only contribute essentially to high moments (like the heat flux) of the distribution function, but are also of particular importance for wall sputtering. Finally, in Sec. IV we summarize our conclusions.

II. SELF-SIMILAR VARIABLES IN A SIMPLE CX MODEL

1. The kinetic equation in self-similar variables

The Boltzmann equation for neutral atoms, interacting with a background plasma through CX, ionization, and recombination is in steady state[1-3]

$$v_{//}\nabla_{//}f_n(\mathbf{v}) = \int \sigma(|\mathbf{v} - \mathbf{v'}|)|\mathbf{v} - \mathbf{v'}|\left[f_i(\mathbf{v})f_n(\mathbf{v'}) - f_n(\mathbf{v})f_i(\mathbf{v'})\right]d^3v' - K_z n_i f_n(\mathbf{v}) + v_r f_i(\mathbf{v}), \quad (1)$$

where f_n and f_i denote the neutral and ion distribution functions, respectively. The first term on the right-hand side describes CX, the second one ionization with the rate constant K_z, and the third term represents a source of neutrals through recombination of ions and electrons with the frequency v_r. As in earlier works, we have neglected neutral-neutral collisions and other processes which may be important in very weakly ionized plasmas. We have also restricted our attention to one spatial dimension in the direction of the gradients of the background plasma; $v_{//}$ denotes the component of the velocity $\mathbf{v}$ in this direction.

The CX cross section is usually[1,2,4-7] taken to be inversely proportional to $|\mathbf{v} - \mathbf{v'}|$, since the CX operator is then greatly simplified. Indeed, if $K_x \equiv \sigma(|\mathbf{v} - \mathbf{v'}|)|\mathbf{v} - \mathbf{v'}|$ is the CX rate constant, Eq. (1) then gives

$$v_{//}\frac{\partial f_n}{\partial y} + f_n = \frac{nK_x + v_r}{n_i(K_x + K_z)}f_i, \quad (2)$$

where n and n_i are the neutral and ion densities, respectively, and $\partial/\partial y \equiv [n_i(K_x+K_z)]^{-1}\nabla_{//}$.

Eqs. (1) and (2) contain several length scales, namely, the mean-free paths with respect to the atomic processes, and the macroscopic length scales associated with the ion distribution function, most importantly those of density and temperature variation. If the ratio of the mean-free paths to the macroscopic lengths is constant throughout the plasma, it is natural to assume that f_n have self-similar structure.[9] Let us therefore seek solutions of the form

$$f_n(y, \mathbf{v}) = \frac{N}{T^\alpha(y)}F(\mathbf{u}), \quad (3)$$

where $u \equiv v / v_T$ is the velocity normalized to the thermal speed at the temperature $T(y)$, $v_T \equiv (2T/M)^{1/2}$, α is a free parameter, and N is a normalization constant chosen such that

$$\int F(\mathbf{u}) \, d^3 u = 1. \tag{4}$$

The neutral density then becomes

$$n(y) = \frac{N v_T^3(y)}{T^\alpha(y)} \propto T^{3/2-\alpha} \tag{5}$$

Eq. (2) now takes the form

$$\gamma \chi u \left(\frac{u}{2} \frac{\partial F}{\partial u} + \alpha F \right) - F = -\beta \hat{f}, \tag{6}$$

where $\chi \equiv u_{//} / u$, $\hat{f} \equiv f_i / \left(n_i v_T^3 \right)$,

$$\beta \equiv \frac{K_x + \nu_r / n}{K_x + K_z}, \tag{7}$$

and

$$\gamma \equiv v_T \frac{d \ln T}{dy} = \frac{v_T}{n_i (K_x + K_z)} \nabla_{//} \ln T = \frac{\lambda_{xz}}{L} \tag{8}$$

is the ratio of the mean-free path λ_{xz} with respect to CX and ionization to the temperature length scale L. For definiteness we shall assume that $\gamma > 0$ so that the temperature increases with y. On the other hand, note that the density of neutrals (5) decreases with y (if $\alpha > 3/2$), whereas their temperature follows that of the ions due to the coupling through CX. In the

following, the solutions of the kinetic equation we obtain thus describe the penetration of neutrals atoms into an increasingly hotter plasma.

If β and γ are both constant, and if $\hat{f}$ depends only on $\mathbf{u}$, then the neutral distribution function is self-similar in y and can be obtained by solving the simple ordinary differential equation (6).[10] The requirement that γ be constant imposes a restriction on the allowed background plasma profiles; the density and ion temperature profiles are coupled through Eq. (8), but one of these profiles is still completely arbitrary. The parameter β is constant if K_z and ν_r/n are constant. These quantities are dependent on the *electron* temperature, and their constancy therefore imposes no additional constraint on T(y). The ionization rate constant K_z is a slowly varying function of the electron temperature above about 20 eV. In order for the quantity ν_r/n to be constant, the recombination rate must decrease with increasing y, i.e., in the direction of increasing temperature, which is indeed the case. Thus, although the requirement that β,γ=const., unfortunately, restricts the applicability of the self-similar solutions somewhat, it does not in any way impose unphysical constraints.

2. The distribution function

Let us now proceed to study the solution to Eq. (6), which is

$$
F(\mathbf{u}) = \begin{cases} \dfrac{2\beta}{\gamma u_{//}} \displaystyle\int_0^1 \hat{f}\left(\dfrac{\mathbf{u}}{s}\right) \exp\left[\dfrac{2(s-1)}{\gamma u_{//}}\right] \dfrac{ds}{s^{2\alpha}}, & u_{//} > 0 \\[4mm] -\dfrac{2\beta}{\gamma u_{//}} \displaystyle\int_1^\infty \hat{f}\left(\dfrac{\mathbf{u}}{s}\right) \exp\left[\dfrac{2(s-1)}{\gamma u_{//}}\right] \dfrac{ds}{s^{2\alpha}}, & u_{//} < 0 \end{cases} . \tag{9}
$$

In addition, there are homogeneous solutions for $u_{//}>0$ proportional to $\exp[-2/(\gamma u_{//})]/u^{2\alpha}$, which are disregarded as being unphysical (representing a tail of hot neutrals originating

from the cold plasma region $y \to -\infty$). If the mean-free path is short, $\gamma \to 0$, the neutral distribution (9) becomes proportional to the ion distribution,

$$\lim_{\gamma \to 0} F(\mathbf{u}) = \beta \, \hat{f}(\mathbf{u}), \tag{10}$$

and not necessarily to a Maxwellian since there is nothing that randomizes particle motion in the kinetic equation (1). Usually, however, we expect the ion distribution to be Maxwellian, $\hat{f}(\mathbf{u}) = \pi^{-3/2} \exp\!\left(-u^2\right)$, which we, for simplicity, take to be at rest. With this choice for the ion distribution, let us consider the neutral distribution over parallel velocities. From Eq. (9) we have

$$F_{//}\!\left(u_{//}\right) \equiv \int F(\mathbf{u}) \, d^2 u_\perp = \begin{cases} \dfrac{2\beta}{\gamma \pi^{1/2} u_{//}} \displaystyle\int_0^1 \exp\!\left[\dfrac{2(s-1)}{\gamma u_{//}} - \dfrac{u_{//}^2}{s^2} \right] \dfrac{ds}{s^{2\alpha - 2}} \,, & u_{//} > 0 \\[2em] -\dfrac{2\beta}{\gamma \pi^{1/2} u_{//}} \displaystyle\int_1^\infty \exp\!\left[\dfrac{2(s-1)}{\gamma u_{//}} - \dfrac{u_{//}^2}{s^2} \right] \dfrac{ds}{s^{2\alpha - 2}} \,, & u_{//} < 0 \end{cases} \tag{11}$$

The first of these expressions has the following asymptotic form

$$F_{//}\!\left(u_{//}\right) \approx \frac{\beta \exp\!\left(-u_{//}^2\right)}{\pi^{1/2}\left[1 - (\alpha - 1)\gamma u_{//} + \gamma u_{//}^3\right]} \,, \quad u_{//} > 0 \tag{12}$$

in the limit $1/\gamma u_{//} + u_{//}^2 - \alpha \gg 1$, which is approached for both small and large $u_{//}$. If the mean-free path is short, this inequality is satisfied for all $u_{//} > 0$. In this case, Eq. (12) is a good approximation for the entire $u_{//} > 0$ part of the distribution function, providing kinetic information to the first order in γ beyond the fluid limit. In particular, we note that $F_{//}(u_{//})$ peaks for

$$\partial F_{//}/\partial u_{//} = 0 \Rightarrow u_{//} \approx \gamma(\alpha-1)/2, \tag{13}$$

and decays much faster than a Maxwellian at high velocities $u_{//} > \gamma^{-1/3}$. The reason for this tail depletion is that particles in this far end of the distribution originate from colder regions (small y). Conversely, for particles traveling in the negative direction ($u_{//} < 0$), the tail is enhanced as compared with a Maxwellian. For $-u_{//} > \gamma^{-1/3} \gg 1$, the asymptotic form of Eq. (11) is

$$F_{//}\left(u_{//}\right) \approx \frac{2\beta}{\pi^{1/2}\gamma^{(2\alpha-1)/3}u_{//}^{2\alpha-2}} \exp\left(-\frac{3}{\gamma^{2/3}} - \frac{2}{\gamma u_{//}}\right), \tag{14}$$

which at large negative velocities approaches a power-law tail, $F_{//}(u_{//}) \propto u_{//}^{-2\alpha-2}$, of particles originating from the hot region $y \to \infty$. Note that the tail is exponentially small in γ, and thus cannot be found by means of any expansion in this parameter, even if indeed $\gamma \ll 1$. Fig. 1 shows a graph of a numerical evaluation of Eq. (11) along with the asymptotic forms (12) and (14). The asymmetric nature of the distribution function is evident with a peak at $u_{//} > 0$, a rapid decay for large positive $u_{//}$, and an elongated tail for negative $u_{//}$.

3. Fluxes

Let us now evaluate the particle flux and the heat flux associated with the neutral distribution function (9). The former,

$$j_{//} \equiv \int f_n v_{//} d^3v = n v_T \int F_{//} u_{//} \, du_{//} \tag{15}$$

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can be obtained directly from the self-similar kinetic equation (6) by integrating it over velocity space, giving

$$j_{//} = \frac{1-\beta}{\gamma(\alpha-2)} n v_T,$$
(16)

regardless of the ion distribution. However, it should be noted that only two of the three parameters α, β and γ are independent since Eq. (4) imposes a constraint on the solution (9). If, for instance, the ion distribution is Maxwellian, Eqs. (4) and (9) imply

$$P(\gamma,\alpha) \equiv \frac{2}{\gamma \pi^{1/2}} \int_0^\infty \frac{du_{//}}{u_{//}} \int_0^\infty \exp\left(-\frac{2|s-1|}{\gamma u_{//}} - \frac{u_{//}^2}{s^2}\right) \frac{ds}{s^{2\alpha}} = \frac{1}{\beta},$$
(17)

which determines one of the three parameters, and the particle flux (16), as a function of the two other parameters. For $\gamma \ll 1$, $P(\gamma,\alpha) \approx 1 + (\alpha-2)(\alpha-5/2)\gamma^2/2$, so the short-mean-free-path limit of Eq. (16) is

$$j_{//} = \frac{\gamma(\alpha-5/2)}{2} n v_T,$$
(18)

in agreement with fluid theory. Indeed, one recovers exactly this result by using Eqs. (5) and (8) in the momentum equation

$$-\nabla_{//}(nT) + M n_i (K_x + K_z) j_{//} = 0$$
(19)

from Ref. 2.

Going beyond the fluid approximation, we can obtain the particle flux from Eq. (16) by evaluating the integrals (17) numerically. Fig. 2 shows the flux normalized to the fluid result (18) close to the singularity at $\alpha=2$ in Eq. (16). The fluid approxiamation is, apparently, not bad unless α is very close to 2, or the mean-free path is very long. When $\alpha \leq 2$, the integral (15) diverges, and the flux becomes infinite. The reason for this is the presence of the high-energy tail $\sim u_{//}^{-2\alpha-2}$, cf. Eq. (14). Unless the neutral density (5) falls off quickly enough with y (i.e., α is sufficiently large), the tail is large enough to dominate the flux, no matter how short the mean-free path is. If $\alpha=5/2$ and $\gamma \to 0$, the flow of hot neutrals from $y \to \infty$ exactly balances the positive particle flux of thermal ones. At large α, the neutral density gradient becomes increasingly steeper [cf. Eq. (5)], and the mean-free path is not adequately measured by γ, which relates only to the temperature gradient. For a comparison of the particle flux with the fluid approximation in this regime, it is therefore more appropriate to plot the ratio as a function of $\gamma\alpha$, as has been done in Fig. 3. The fluid result is quite good, even for moderate mean-free paths, $\gamma\alpha<1$, unless α becomes very large. In this limit ($\alpha \to \infty$, but $\gamma\alpha$ remaining finite), Eq. (17) implies that $\beta \to 0$, and the ratio of the actual flux (16) to fluid result (18) approaches $2/(\gamma\alpha)^2$ (the dotted line). The approach to this asymptote is slow for small values of $\gamma\alpha$; a detailed analysis shows that it occurs if $\alpha > (\gamma\alpha)^{-2}$. Physically, the limit $\beta \to 0$ means that ionization dominates over CX and recombination [cf. Eq. (7)], in which case the fluid limit cannot be realized since the neutral-ion coupling through CX disappears.

This effect of the tail is, of course, even more pronounced in higher moments of the distribution, as in the heat flux

$$q_{//} \equiv \int f_n \frac{Mv^2}{2} v_{//} d^3v = v_T nT \int F u^2 u_{//} \, du_{//} . \tag{20}$$

Substituting the solution (9) into (20) gives

$$q_{//} = v_T nT \frac{2\beta}{\gamma} \int_0^\infty \left(\tau + u_{//}^2\right) du_{//}$$

$$\times \left\{ \int_0^1 \hat{f}_{//}\left(u_{//}\right) \exp\left[\frac{2(s-1)}{\gamma u_{//} s}\right] \frac{ds}{s^{2\alpha-5}} - \int_1^\infty \hat{f}_{//}\left(-u_{//}\right) \exp\left[\frac{2(1-s)}{\gamma u_{//} s}\right] \frac{ds}{s^{2\alpha-5}} \right\} \quad (21)$$

if the ion distribution can be written as $\hat{f}(\mathbf{u}) = \hat{f}_\perp(\mathbf{u}_\perp)\hat{f}_{//}(\mathbf{u}_{//})$, where $\int \hat{f}_\perp(\mathbf{u}_\perp) d^2 u_\perp \equiv 1$, and τ is the normalized perpendicular temperature

$$\tau \equiv \int \hat{f}_\perp(\mathbf{u}) u_\perp^2 d^2 u_\perp . \qquad - \qquad (22)$$

In the limit $\gamma \to 0$, Eq. (21) reduces to

$$q_{//} \approx v_T nT\beta \left[\int_{-\infty}^\infty \left(\tau + u_{//}^2\right) u_{//} \hat{f}_{//}\left(u_{//}\right) du_{//} + \gamma(2\alpha - 7) \int_{-\infty}^\infty \left(\tau + u_{//}^2\right) u_{//}^2 \hat{f}_{//}\left(u_{//}\right) du_{//} \right], \quad (23)$$

and for Maxwellian ions we obtain

$$q_{//} \xrightarrow{\gamma \to 0} \gamma \frac{5(\alpha - 7/2)}{4} \beta v_T nT , \qquad (24)$$

in agreement with Eq. (67) of Ref. 2, according to which the conductive part of the heat flux is

$$q_{cond} = -\frac{5nT}{2Mn_i\left(K_x + K_z\right)} \nabla_{//} T . \qquad (25)$$

Using Eq. (8) for $\nabla_{//}T$ and adding the convective heat flux corresponding to the flow (18) gives precisely (24). Apparently, when $\alpha=7/2$, the convective and conductive parts of the heat flux cancel exactly in the fluid limit. If γ is finite, the heat flux can be obtained by evaluating Eq. (21) numerically. Choosing the ions to be Maxwellian, we see from Fig. 4 that the fluid result is not bad unless α is very close to the value where the tail particles dominate, which now occurs at $\alpha=3$. If $\alpha\leq3$, the second integral in Eq. (21) diverges as the flux associated with the tail becomes infinite, again regardless of the mean-free path. For $\alpha<4$, the heat flux increases more slowly than linearly for large γ. This can be understood by taking the limit $\gamma\rightarrow\infty$ in Eq. (21), which for Maxwellian ions becomes

$$q_{//} \xrightarrow{\gamma\rightarrow\infty} \gamma^{2\alpha-7} v_T nT \beta \frac{(\alpha-3/2)\Gamma(\alpha-5/2)\Gamma(2\alpha-6)}{2^{2\alpha-6}\pi^{1/2}} \qquad (26)$$

The curves in Fig. 4 have $\alpha<4$ and therefore decrease for large γ. For large values of α, Fig. 5 shows that the fluid result is again quite good unless α or the normalized mean-free path $\gamma\alpha$ becomes very large.

III. A MORE EXACT MODEL FOR CX

The high-energy tail discussed in the previous section consists of fast neutrals that have escaped from the hot region $y\rightarrow\infty$. This is possible since the mean-free path increases with energy. Indeed, the assumption that $\sigma\propto 1/v_{rel}$ made in the previous section and in most earlier works[1,2,4-7] gives a mean free path that increases linearly with velocity, $\lambda=<\sigma v_{rel}>v_{rel}=K_x v_{rel}$. In reality, σ depends much more weakly on the velocity. In the present section, we employ the much more exact model

$$\sigma(v_{rel}) = \sigma_0 v_{rel}^{\delta-1}, \qquad (27)$$

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where $\delta \approx 0.84$, shown in Fig. 6 along with the exact cross section taken from Ref. 11. The conventional model is recovered by letting $\delta = 0$, and the approximation $\sigma = $ constant, used for deriving fluid equations in Ref. 3, is obtained in the limit $\delta \to 1$.

With the CX cross section (27), the kinetic equation (1) again has self-similar solutions if simplifying assumptions are made about the ionization and recombination rates. Indeed, if the ionization rate constant is

$$K_z(T) = \zeta v_T \sigma(v_T), \qquad \qquad (28)$$

and the quantities ζ, $\gamma \equiv d(\ln T)/dy \equiv [n_i \sigma(v_T)]^{-1} \nabla_{//}(\ln T)$ and

$$\rho \equiv \frac{\nu_r}{n n_i v_T \sigma(v_T)} \qquad \qquad (29)$$

are constant, we can make the self-similar Ansatz (3) and write Eq. (1) as

$$-\gamma \chi u \left(\frac{u}{2} \frac{\partial F}{\partial u} + \alpha F \right) = \int |u - u'|^\delta \left[\hat{f}(u)F(u') - \hat{f}(u')F(u) \right] d^3 u' - \zeta F + \rho \hat{f}. \qquad (30)$$

It is clear that if $\hat{f}$ only depends on u, then so does the solution F to Eq. (30), i.e., it has self-similar structure.

Eq. (30) is still too difficult to solve analytically because of the complicated form of the CX operator. However, if we only consider tail particles, we may take $u \gg u'$ in the CX operator, simplifying Eq. (30) to

$$\gamma\chi u\left(\frac{u}{2}\frac{\partial F}{\partial u}+\alpha F\right)-\left(u^\delta+\zeta\right)F=-\left(u^\delta+\rho\right)\hat{f}. \tag{31}$$

For particles traveling in the negative ($\chi<0$) direction, the solution to this equation is

$$F(\mathbf{u})=-\frac{2}{\gamma\chi u^2}\int_0^u\left(\frac{u'}{u}\right)^{2(\alpha-1)}\left(u'^\delta+\rho\right)\exp\left[\frac{2}{\gamma\chi}\left(\frac{\zeta}{u'}-\frac{\zeta}{u}+\frac{u'^{\delta-1}-u^{\delta-1}}{1-\delta}\right)\right]\hat{f}(u')du' \tag{32}$$

for $0<\delta<1$, and

$$F(\mathbf{u})=-\frac{2}{\gamma\chi u^2}\int_0^u\left(\frac{u'}{u}\right)^{2(\alpha-1)-1/\gamma\chi}\left(u'^\delta+\rho\right)\exp\left[\frac{2}{\gamma\chi}\left(\frac{\zeta}{u'}-\frac{\zeta}{u}\right)\right]\hat{f}(u')du' \tag{33}$$

for $\delta=1$. In these integrals, the direction of $\mathbf{u}'$ is to be held constant in the integration; only its magnitude u' varies. One important difference between Eqs. (32) and (33) is seen immediately: If $\delta<1$, the distribution function has a tail proportional to $u^{-2\alpha}$, as in the previous section, whereas if $\delta=1$, the tail is extremely small for short mean-free paths, being proportional to only $u^{-(2\alpha-1/\gamma\chi)}$, where the exponent is $2\alpha-1/\gamma\chi\gg1$. The underlying physical reason for this is that if $\delta=1$, the CX cross section and therefore also the mean-free path are independent of velocity. Consequently, fast neutral are no more able than slow ones to escape from the hot region $y\to\infty$.

Since actually $\delta\approx0.84$, an sizable tail arises consisting of fast neutrals traveling in the negative direction. The asymptotic form of the distribution function (32) is

$$F(\mathbf{u})\approx\frac{2u_*^{1-\delta}\left(u_*^\delta+\rho\right)}{\pi\sqrt{3-\delta}}\left(\frac{u_*}{u}\right)^{2\alpha}\exp\left[Q(u,u_*)\right], \tag{34}$$

where

$$Q(u, u_*) \equiv \frac{2}{\gamma\chi}\left(\frac{\zeta}{u_*} - \frac{\zeta}{u} + \frac{u_*^{\delta-1} - u^{\delta-1}}{1-\delta}\right) - u_*^2,$$ (35)

and u_* is defined as the value of u' where the exponent in Eq. (32) peaks,

$$u_* \approx \frac{1}{(-\gamma\chi)^{1/(3-\delta)}}\left[1 + \frac{\zeta}{3-\delta}(-\gamma\chi)^{\delta/(3-\delta)}\right].$$ (36)

In the far tail region, $u \gg u_* \gg 1$, the distribution (34) has the form $F(u,\chi)=F_0(\chi)/u^{2\alpha}$. Again, the height of the tail is non-expandable in γ, and the moments corresponding to the particle flux (15) or the heat flux (20) still diverge for $\alpha \leq 2$ and $\alpha \leq 3$, respectively. The effect of the tail on the fluxes is thus qualitatively the same as in the simpler model $\delta=0$ considered in the previous section. The shape of the tail is also important for wall sputtering, which in some cases can be dominated by fast neutrals escaping from the hot plasma and reaching the wall. Our analysis shows that the tail should be expected to be strongly enhanced over an Maxwellian, as was also pointed out in Ref. 8.

IV. CONCLUSIONS

The results of this paper can be summarized as follows:

1. If the density and temperature gradients are constant *as measured in neutral mean-free paths*, there are self-similar solutions to the Boltzmann equation for neutral atoms in a plasma undergoing CX, ionization, and recombination. These solutions describe neutrals penetrating into a hot plasma.

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2. If the usual assumption is made that the CX cross section is inversely proportional to the relative velocity, it is possible to find the exact self-similar solutions analytically for arbitrary mean-free paths. The neutral distribution function is markedly asymmetric with a peak at positive velocities, and a power-law tail at large negative velocities. In a more accurate model with the CX cross section decreasing as a (small) power of the relative velocity, $\sigma(v_{rel}) = \sigma_0 v_{rel}^{\delta-1}$, the tail persists and has qualitatively the same structure. It is non-expandable in γ, and therefore eludes any short-mean-free-path expansion.

3. The self-similar solutions can be used to test the accuracy of neutral fluid models, currently in use, e.g., in plasma edge codes,[12,13] and to benchmark Monte Carlo codes.[14] Most importantly, the kinetic and fluid predictions for the fluxes of heat and particles can be compared. This comparison shows that the requirement that the mean-free path be short is *not* sufficient for the fluid results to be correct. In addition, the parameter α in Eq. (5), which is determined by the mean-free path and the rate constants of the atomic processes, must be large enough. For instance, if $\alpha \leq 3$ the expression (21) for the heat flux diverges because of the power-law tail in the distribution function. Of course, the heat flux does not actually become infinite, since the tail is limited by the circumstance that the extent of the plasma, as well as its temperature, is bounded. Some cut-off therefore appears in the diverging integral. The point is, however, that the heat flux can become extremely large before this happens; since there are usually big temperature differences in the plasma, $T_{max} \gg T_{min}$, the cut-off appears only at very high energy. The mean-free path must therefore be exceedingly small to ensure the correctness of the fluid approximation in this case. On the other hand, if the tail does not the dominate the fluxes, or if T_{max}/T_{min} is moderate so the tail does not exist, fluid results appear to be quite accurate even for relatively large values ($\gamma\alpha < 1$) of the mean-free path.

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[12]S.I. Krasheninnikov, A.S. Kukushkin, and V.A. Pozharov, *11th International Conference on Plasma Physics and Controlled Nuclear Fusion Research* (IAEA, Vienna, 1987). Vol. 2, p. 177.

[13]D.A. Knoll, P.R. McHugh, S.I. Krasheninnikov, and D.J. Sigmar, *Simulation of dense recombining divertor plasmas with a Navier-Stokes neutral transport model*, submitted to Phys. Plasmas.

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FIGURE CAPTIONS

Fig. 1. The neutral distribution function (11) over parallel velocity divided by β (bold line), and its asymptotic forms from Eqs. (12) and (14) (dotted lines). The former [Eq. (12)] almost coincides with the bold line. $\alpha=4$, $\gamma=0.2$.

Fig. 2. The neutral particle flux (16) normalized to that in the fluid limit (18) vs γ for α ranging from 2.03 to 2.2.

Fig. 3. The neutral particle flux (16) normalized to that in the fluid limit (18) vs $\gamma\alpha$ for large α (bold lines), and the asymptotic limit $\alpha\rightarrow\infty$ (dashed line).

Fig. 4. The neutral heat flux (23) with Maxwellian ions normalized to that in the fluid limit (24) vs γ for α from 3.03 to 3.2.

Fig. 5. The neutral heat flux (23) with Maxwellian ions normalized to that in the fluid limit (18) vs $\gamma\alpha$.

Fig. 6. The CX cross section[11] σ (bold line) for hydrogen vs relative kinetic energy, and the approximation (27) (dotted line).
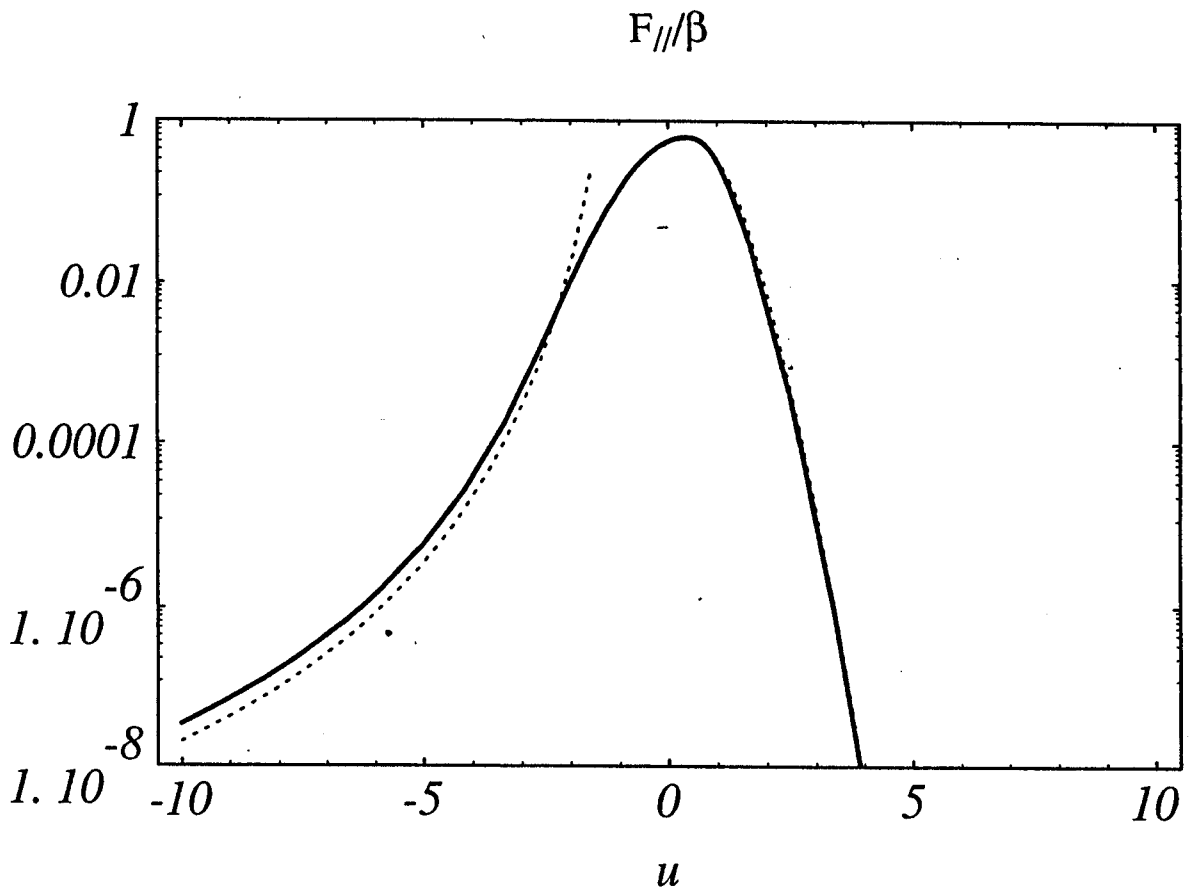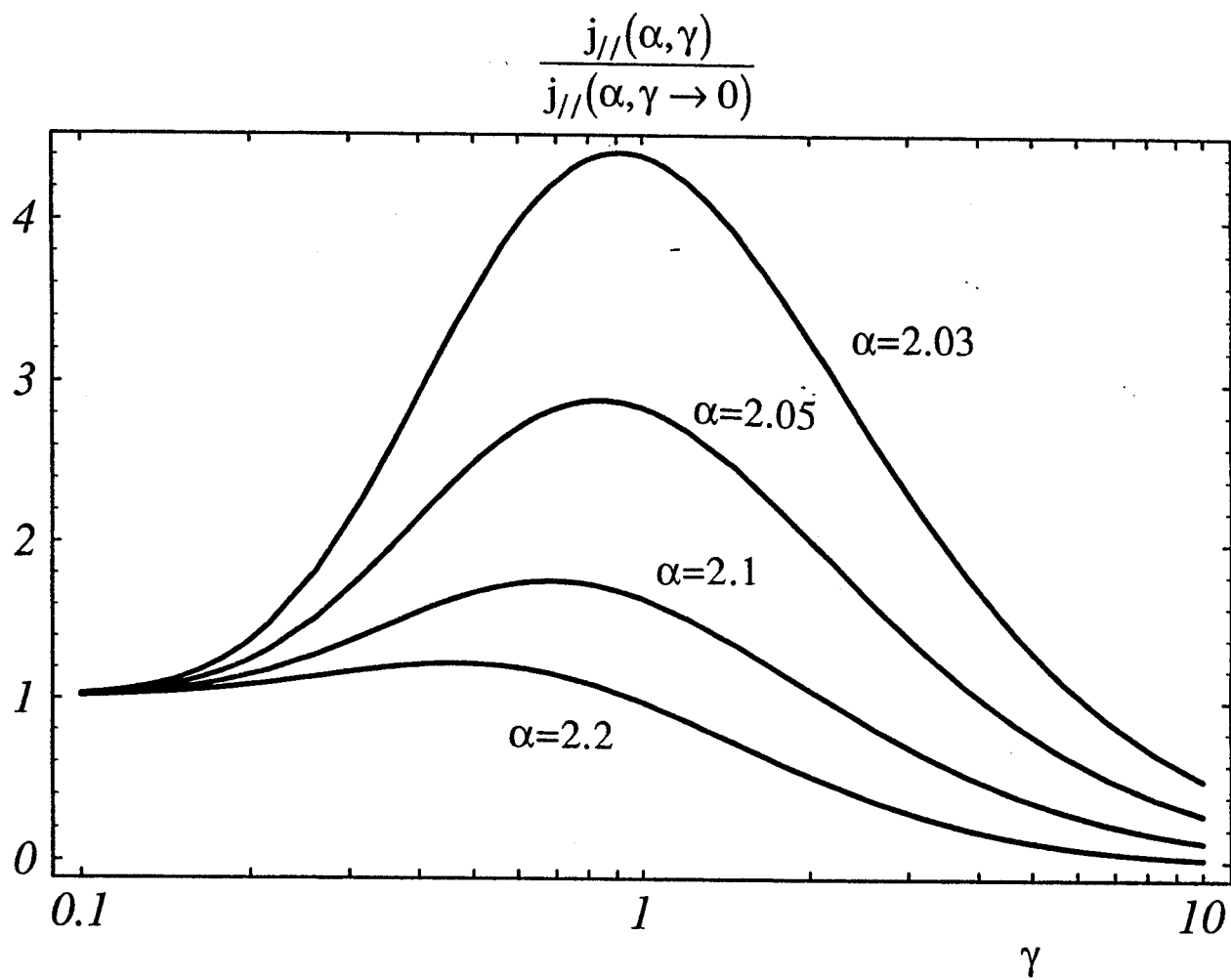
$F_{///}\beta$

u

Fig. 1

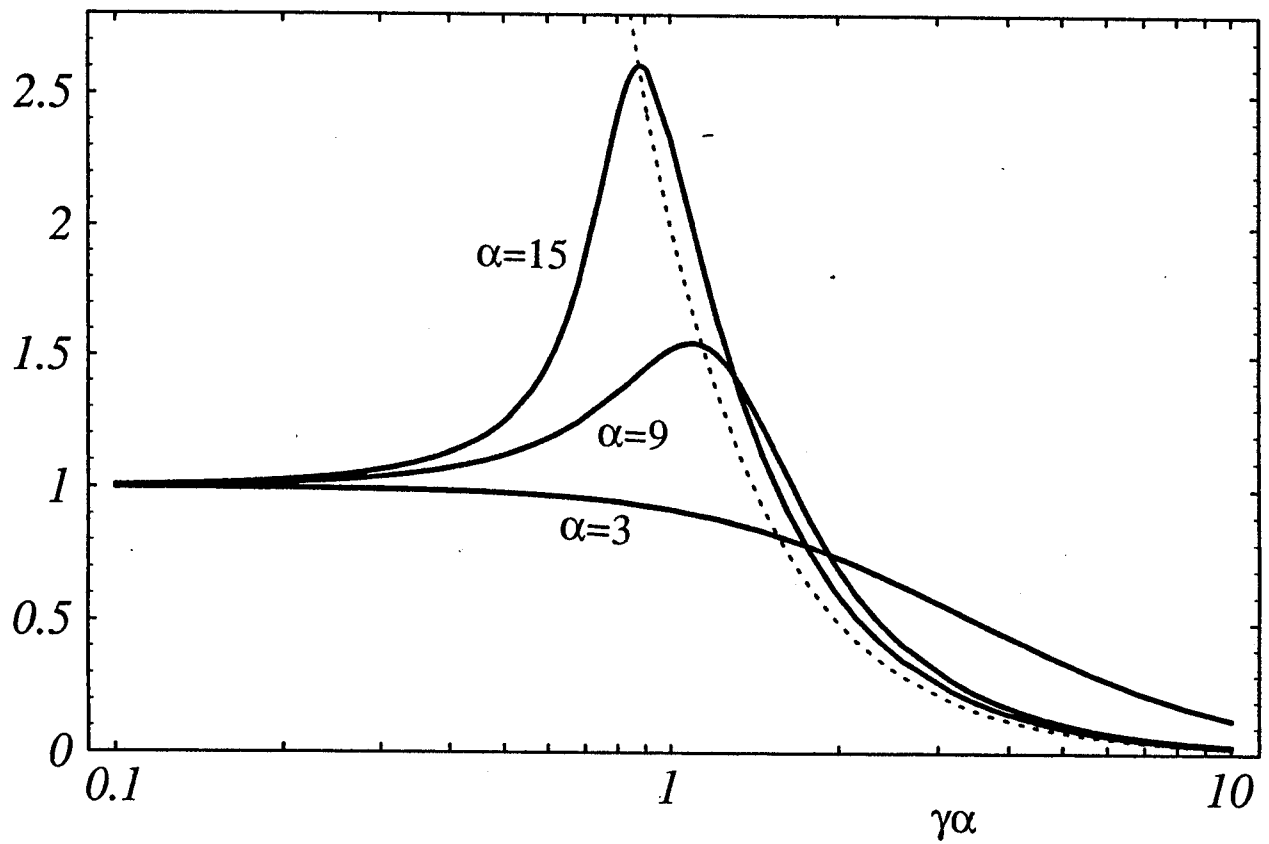$$\frac{j_{//}(\alpha, \gamma)}{j_{//}(\alpha, \gamma \to 0)}$$

α=2.03

α=2.05

α=2.1

α=2.2

γ

Fig. 2

$$\frac{j_{//}(\alpha,\gamma)}{j_{//}(\alpha,\gamma \to 0)}$$

α=15

α=9

α=3

γα

Fig. 3

$$\frac{q_{//}(\alpha,\gamma)}{q_{//}(\alpha,\gamma \to 0)}$$

α=3.03

α=3.05

α=3.1

α=3.2

γ

Fig. 4

$$\frac{q_{//}(\alpha,\gamma)}{q_{//}(\alpha,\gamma \to 0)}$$

$\alpha=10$

$\alpha=6$

$\alpha=5$

$\alpha=4$

$\gamma\alpha$

Fig. 5

$$\frac{\sigma}{10^{-19}\,m^2}$$

Energy (eV)

Fig. 6