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The Transport of Neutral Hydrogen Atoms in a Hydrogen Plasma

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Abstract—*An analytical version of the discrete ordinates method is used to solve a class of boundary-value problems based on a linear Boltzmann equation relevant to the transport of neutral hydrogen atoms in a hydrogen plasma. In addition to a complete development of the discrete ordinates method for the considered application, the computational algorithm is implemented to yield very accurate results for a number of half-space and finite-slab problems. The developed code is also used to correct some entries in a previously reported tabulation of results. The established algorithm is considered especially easy to use, and the code runs (typically) in <1 s on a 400-MHz Pentium-based personal computer.*

I. INTRODUCTION

In this work, we consider the transport of neutral particles in a plasma that, as pointed out by Tendler and Heifetz,[1] is a subject of concern in fusion research. It was also noted, in Tendler and Heifetz's review paper[1] on neutral particle kinetics in fusion devices, that knowledge of the distribution of neutral particles in a plasma is important in analyzing the energy balance in the plasma and the role played by the neutrals in the mechanism of plasma refueling and exhaust, in estimating the damage to the device walls, and in the designing of diagnostic tools.

Since there are situations in plasma physics where the neutral mean free path in the plasma can be comparable to the plasma scale length, the Boltzmann equation (rather than low-order fluid equations) is usually required for modeling the physics of the problem accurately. Early kinetic models have been put forward by Sakharov,[2] Zubarev and Klimov,[3] and Konstantinov and Perel.[4] In the following years, more sophisticated models and methods of solution for the ensuing Boltzmann equations were reported in the literature. The models evolved to consider the more realistic cases of multiple neutral species, a spatially dependent ion temperature, and a combination of specular and diffuse reflection at the wall. In regard to techniques for analyzing the various models used to describe the transport of neutral atoms in a plasma, we note that analytical, semianalytical, numerical, and stochastic methods have all been investigated, and since both the important models and the important transport techniques relevant to this work have been thoroughly reviewed in Ref. 1, we do not address these issues here.

In this work, we use an analytical version of the discrete ordinates method recently developed and used to solve problems in radiative transfer,[5–7] neutron transport,[8] and rarefied gas dynamics[9–11] to study the transport of neutral hydrogen atoms in a hydrogen plasma. We consider both half-space and finite-slab problems with spatially constant ion temperatures and different amounts of specular and diffuse reflection at the walls upon which neutral particles are incident. We also implement the developed solution to obtain especially accurate numerical results that are compared to our F_N results that were reported, for this class of problems, a few years ago in a joint work with Pomraning.[12]

II. THE TRANSPORT EQUATION AND BOUNDARY CONDITIONS

We base our development in this section on the equivalent material that was formulated (almost exclusively by Pomraning) in our previous work[12] on this subject. The steady-state Boltzmann equation that describes the transport of low-energy (<5-keV) neutral hydrogen atoms in a hydrogen plasma can be written as[12]

$$\mathbf{v}\cdot\nabla f_0(\mathbf{r},\mathbf{v}) + \sigma(\mathbf{r},\mathbf{v}) f_0(\mathbf{r},\mathbf{v}) = f_i(\mathbf{r},\mathbf{v}) \int_{\mathbf{v}'} |\mathbf{v}-\mathbf{v}'|\sigma_x(|\mathbf{v}-\mathbf{v}'|) f_0(\mathbf{r},\mathbf{v}')\,\mathrm{d}\mathbf{v}' \ , \quad (1)$$

where

$$\sigma(\mathbf{r},\mathbf{v}) = \int_{\mathbf{v}'} |\mathbf{v}-\mathbf{v}'|[\sigma_e(|\mathbf{v}-\mathbf{v}'|) f_e(\mathbf{r},\mathbf{v}') + \sigma_x(|\mathbf{v}-\mathbf{v}'|) f_i(\mathbf{r},\mathbf{v}')]\mathrm{d}\mathbf{v}' \ , \quad (2)$$

and where $f_0(\mathbf{r},\mathbf{v})$, $f_e(\mathbf{r},\mathbf{v})$ and $f_i(\mathbf{r},\mathbf{v})$ are, respectively, the neutral, electron and ion distribution functions, and $\sigma_e(v)$ and $\sigma_x(v)$ are the cross sections for electron ionization and charge exchange. In Ref. 12, it was noted that Eq. (1) can be simplified if we use the experimental result that the charge-exchange cross section varies approximately with the inverse of the speed and if, considering the large difference in mass between the electron and the hydrogen atom, we take the ionization rate to be independent of the neutral velocity. We therefore rewrite Eq. (1) as

$$\mathbf{v}\cdot\nabla f_0(\mathbf{r},\mathbf{v}) + N_i(\mathbf{r})(\langle\sigma_x v\rangle + \langle\sigma_e v\rangle) f_0(\mathbf{r},\mathbf{v}) = N_i(\mathbf{r})\langle\sigma_x v\rangle f_n(\mathbf{r},\mathbf{v}) \int_{\mathbf{v}'} f_0(\mathbf{r},\mathbf{v}')\,\mathrm{d}\mathbf{v}' \ , \quad (3)$$

where $N_i(\mathbf{r})$ is the ion density, which we assume to be the same as the electron density by imposing charge neutrality, $f_n(\mathbf{r},\mathbf{v}) = f_i(\mathbf{r},\mathbf{v})/N_i(\mathbf{r})$ is a spatially normalized ion distribution, and the $\langle\cdots\rangle$ notation means that an average has been taken over the appropriate electron or ion distribution. We note that in the case of the quantity $\sigma_x v$, the averaging notation is superfluous since, as mentioned before, $\sigma_x(v) \propto 1/v$ and therefore $\sigma_x v$ is constant.

In the approach to the reactor regime, the density and the size of the plasma increase, and the neutrals are confined to a relatively narrow surface layer, and so it makes sense to specialize Eq. (3) to plane geometry. This allows us to integrate the resulting equation over v_x and v_y (two of the components of the velocity $\mathbf{v}$) to obtain

$$v_z \frac{\partial}{\partial z} g_0(z,v_z) + N_i(z)(\langle\sigma_x v\rangle + \langle\sigma_e v\rangle) g_0(z,v_z) = N_i(z)\langle\sigma_x v\rangle g_n(z,v_z) \int_{-\infty}^{\infty} g_0(z,v_z')\,\mathrm{d}v_z' \ , \quad (4)$$

where we have defined, for $\alpha = 0$ or $\alpha = n$,

$$g_\alpha(z,v_z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_\alpha(\mathbf{r},\mathbf{v})\,\mathrm{d}v_x \mathrm{d}v_y \ . \quad (5)$$

Introducing the optical variable

$$\tau = (1/\bar{v}) \int_0^z N_i(z')(\langle\sigma_x v\rangle + \langle\sigma_e v\rangle)\,\mathrm{d}z' \ , \quad (6)$$

where $\bar{v}$ is a characteristic speed, and letting $u = v_z/\bar{v}$ and $\psi(\tau,u) \rightarrow g_0(z,v_z)$, we can rewrite Eq. (4) for $u \in (-\infty,\infty)$ as

$$u \frac{\partial}{\partial\tau} \psi(\tau,u) + \psi(\tau,u) = cF(\tau,u) \int_{-\infty}^{\infty} \psi(\tau,u')\,\mathrm{d}u' \ , \quad (7)$$

where

$$c = \frac{\langle\sigma_x v\rangle}{\langle\sigma_x v\rangle + \langle\sigma_e v\rangle} \quad (8)$$

and $F(\tau,u) \rightarrow \bar{v} g_n(z,v_z)$. Usually, $F(\tau,u)$ can be well represented by a local Maxwellian for the ion distribution, namely,

$$F(\tau,u) = \bar{v}[\pi^{1/2} v_i(\tau)]^{-1} \mathrm{e}^{-u^2\bar{v}^2/v_i^2(\tau)} \ , \quad (9)$$

where the thermal speed $v_i(\tau)$ is related to the local ion temperature $T_i(\tau)$ by

$$v_i(\tau) = \left[\frac{2kT_i(\tau)}{m_i}\right]^{1/2} \ . \quad (10)$$

Here, as in Ref. 12, we consider the case where $T_i(\tau)$ and, by extension, $v_i(\tau)$ are independent of τ. Hence, choosing $\bar{v} = v_i$, we can write Eq. (7) as

$$u \frac{\partial}{\partial\tau} \psi(\tau,u) + \psi(\tau,u) = c\pi^{-1/2} \mathrm{e}^{-u^2} \int_{-\infty}^{\infty} \psi(\tau,u')\,\mathrm{d}u' \ . \quad (11)$$

To complete the definition of the problem, we now turn our attention to the boundary conditions subject to which Eq. (11) should be solved. Assuming that the plasma extends from $z = 0$ to $z = z_0$, we follow Ref. 12 and consider, for $z = 0$ and $v_z \in (0,\infty)$,

$$f_0(\mathbf{r}_s,\mathbf{v}) = \gamma_-(\mathbf{v}) + \rho_-^s f_0(\mathbf{r}_s,\mathbf{v}_\mathbf{r}) + \rho_-^d h_-(\mathbf{v}) \times \int_0^\infty \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} v_z' f_0(\mathbf{r}_s,\mathbf{v}_\mathbf{r}')\,\mathrm{d}v_x'\mathrm{d}v_y'\mathrm{d}v_z' \ , \quad (12)$$

where $\mathbf{r}_s = (x,y,0)$, $\mathbf{v}_r = (v_x,v_y,-v_z)$, $\gamma_-(\mathbf{v})$ is a known incident distribution of neutrals, ρ_-^s and ρ_-^d are, respectively, the coefficients of specular and diffuse reflection, and the redistribution function $h_-(\mathbf{v})$ is normalized to a unit partial flux in the positive z direction, that is,

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty v_z h_-(\mathbf{v})\, \mathrm{d}v_x \mathrm{d}v_y \mathrm{d}v_z = 1 \ . \tag{13}$$

We note that in terms of the optical variable τ and the reduced speed u, Eq. (12) yields, for $u \in (0,\infty)$,

$$\psi(0,u) = \Gamma_-(u) + \rho_-^s \psi(0,-u) + \rho_-^d H_-(u) \times \int_0^\infty \psi(0,-u')u'\, \mathrm{d}u' \ , \tag{14}$$

where

$$\Gamma_-(u) = \int_{-\infty}^\infty \int_{-\infty}^\infty \gamma_-(\mathbf{v})\, \mathrm{d}v_x \mathrm{d}v_y \tag{15}$$

and

$$H_-(u) = \bar{v}^2 \int_{-\infty}^\infty \int_{-\infty}^\infty h_-(\mathbf{v})\, \mathrm{d}v_x \mathrm{d}v_y \tag{16}$$

with $H_-(u)$ normalized as

$$\int_0^\infty H_-(u) u\, \mathrm{d}u = 1 \ . \tag{17}$$

At $\tau = \tau_0$, a similarly general boundary condition can be considered. We thus write, for $u \in (0,\infty)$,

$$\psi(\tau_0,-u) = \Gamma_+(u) + \rho_+^s \psi(\tau_0,u) + \rho_+^d H_+(u) \times \int_0^\infty \psi(\tau_0,u')u'\, \mathrm{d}u' \ . \tag{18}$$

To close this section, we note that in the case of a plasma filling the half-space $\tau > 0$, it is clear that instead of Eq. (18), we must consider the condition

$$\lim_{\tau\to\infty} \psi(\tau,u) = 0 \ . \tag{19}$$

III. THE PROBLEMS

In this section, we restate, in strictly mathematical terms, the basic problems that were defined in our earlier work,[12] which are also discussed in Sec. II and which we intend to solve here.

III.A. Half-Space Problems

In regard to Eq. (11), we let

$$Y(\tau,u) = \mathrm{e}^{u^2} \psi(\tau,u) \ , \tag{20}$$

and so, for half-space ($\tau > 0$) applications, we consider our problem to be defined by the (transformed) transport equation

$$u \frac{\partial}{\partial \tau} Y(\tau,u) + Y(\tau,u) = \int_{-\infty}^\infty \Psi(\mu) Y(\tau,\mu)\, \mathrm{d}\mu \tag{21}$$

for $\tau \in (0,\infty)$ and $u \in (-\infty,\infty)$, the condition at infinity, namely,

$$\lim_{\tau\to\infty} Y(\tau,u) = 0 \ , \tag{22a}$$

and the boundary condition

$$Y(0,u) = F(u) + \rho_s Y(0,-u) + \rho_d G(u) \int_0^\infty Y(0,-\mu) \mathrm{e}^{-\mu^2} \mu\, \mathrm{d}\mu \tag{22b}$$

for $u \in (0,\infty)$. Here and throughout this work (what we call) the characteristic function is

$$\Psi(u) = c\pi^{-1/2} \mathrm{e}^{-u^2} \ . \tag{23}$$

We consider that the known (specified) terms in Eq. (22b) can be written as

$$F(u) = \Delta \frac{\mathrm{e}^{u^2}}{u} \delta(u - u_0) + (1-\Delta) 2b \mathrm{e}^{-(b-1)u^2} \tag{24a}$$

and

$$G(u) = 2a \mathrm{e}^{-(a-1)u^2} \ , \tag{24b}$$

where the parameters $a > 0$, $b > 0$, and $u_0 > 0$ are assumed to be given and where the arbitrary constant Δ is used in order to be able simply to include the two boundary conditions ($\Delta = 1$ and $\Delta = 0$) considered in Ref. 12. We note that because of the way the functions $F(u)$ and $G(u)$ are normalized, we can write

$$I^* = 1 + (\rho_s + \rho_d) O^* \ , \tag{25}$$

where the partial fluxes I^* and O^* are defined as

$$I^* = \int_0^\infty Y(0,u) \mathrm{e}^{-u^2} u\, \mathrm{d}u \tag{26a}$$

and

$$O^* = \int_0^\infty Y(0,-u) \mathrm{e}^{-u^2} u\, \mathrm{d}u \ . \tag{26b}$$

And so, in regard to these half-space applications, we intend to use our discrete ordinates method to compute the partial flux O^* for various values of the defining parameters.

III.B. Finite-Slab Problems

For the applications in a finite slab, we again follow Ref. 12 and seek a solution to

$$u \frac{\partial}{\partial \tau} Y(\tau,u) + Y(\tau,u) = \int_{-\infty}^\infty \Psi(\mu) Y(\tau,\mu)\, \mathrm{d}\mu \tag{27}$$

for $\tau \in (0,\tau_0)$ and $u \in (-\infty,\infty)$, subject to the boundary conditions

$$Y(0,u) = F(u) + \rho_s Y(0,-u) + \rho_d G(u) \int_0^\infty Y(0,-\mu) e^{-\mu^2} \mu \, d\mu \quad (28a)$$

and

$$Y(\tau_0,-u) = F(u) + \rho_s Y(\tau_0,u) + \rho_d G(u) \int_0^\infty Y(\tau_0,\mu) e^{-\mu^2} \mu \, d\mu \quad (28b)$$

for $u \in (0,\infty)$. While a nonsymmetric version of Eqs. (28) was defined in Ref. 12, we consider it sufficient, for the purpose of illustrating the fundamental aspects of our discrete ordinates solution, to base our numerical work on the symmetric case. Here, we intend to compute the partial flux

$$O^* = \int_0^\infty Y(0,-u) e^{-u^2} u \, du \quad (29)$$

and the neutral distribution

$$\psi_*(\tau,u) = e^{-u^2} Z(\tau,u) \quad (30)$$

for various values of the defining parameters and selected values of $\tau \in [0,\tau_0]$ and $u \in (-\infty,\infty)$. Here, we use $Z(\tau,u)$ to denote the component of $Y(\tau,u)$ that is not a generalized (delta) function.

IV. THE REDUCED PROBLEMS

Since the boundary conditions listed as Eq. (22b), for the half-space case, and Eqs. (28), for the finite-slab problems, introduce into the desired solutions a component that is a generalized function, we make use of a convenient decomposition of the solution before proceeding with our discrete ordinates method.

IV.A. Half-Space Problems

For half-space applications, we write

$$Y(\tau,u) = \frac{\Delta}{u} e^{u^2} \delta(u-u_0) e^{-\tau/u} + Z(\tau,u) \ , \quad (31)$$

where after substituting Eq. (31) into Eqs. (21) and (22), we see that $Z(\tau,u)$ is defined by the transport equation

$$u \frac{\partial}{\partial \tau} Z(\tau,u) + Z(\tau,u) = \int_{-\infty}^{\infty} \Psi(\mu) Z(\tau,\mu) \, d\mu + Q(\tau) \quad (32)$$

for $\tau \in (0,\infty)$ and $u \in (-\infty,\infty)$, the condition at infinity, namely,

$$\lim_{\tau\to\infty} Z(\tau,u) = 0 \ , \quad (33a)$$

and the boundary condition

$$Z(0,u) = R(u) + \rho_s Z(0,-u) + \rho_d G(u) \int_0^\infty Z(0,-\mu) e^{-\mu^2} \mu \, d\mu \quad (33b)$$

for $u \in (0,\infty)$. We note that the known terms in Eqs. (32) and (33b) are given by

$$Q(\tau) = \frac{\Delta}{u_0} c\pi^{-1/2} e^{-\tau/u_0} \quad (34)$$

and

$$R(u) = (1-\Delta) 2b e^{-(b-1)u^2} \ . \quad (35)$$

Now, making use of Eq. (31), we rewrite Eq. (26b) as

$$O^* = \int_0^\infty Z(0,-u) e^{-u^2} u \, du \ . \quad (36)$$

IV.B. Finite-Slab Problems

Here, to avoid the generalized function in our discrete ordinates solution, we let

$$Y(\tau,u) = Y_0(\tau,u) + Z(\tau,u) \ , \quad (37)$$

where after substituting Eq. (37) into Eqs. (28), we choose to define

$$Y_0(\tau,u) = K(u) e^{-\tau/u} \quad (38a)$$

and

$$Y_0(\tau,-u) = K(u) e^{-(\tau_0-\tau)/u} \ , \quad (38b)$$

where

$$K(u) = \frac{\Delta}{u} T(u) e^{u^2} \delta(u-u_0) \quad (39)$$

and

$$T(u) = (1-\rho_s e^{-\tau_0/u})^{-1} \quad (40)$$

for $u \in (0,\infty)$. Now, if we substitute the decomposition given by Eq. (37) into Eqs. (27) and (28), we find that the required $Z(\tau,u)$ is defined by

$$u \frac{\partial}{\partial \tau} Z(\tau,u) + Z(\tau,u) = \int_{-\infty}^{\infty} \Psi(\mu) Z(\tau,\mu) \, d\mu + Q(\tau) \quad (41)$$

for $\tau \in (0,\tau_0)$ and $u \in (-\infty,\infty)$ and the boundary conditions

$$Z(0,u) = R(u) + \rho_s Z(0,-u) + \rho_d G(u)\int_0^\infty Z(0,-\mu)\mathrm{e}^{-\mu^2}\mu\,\mathrm{d}\mu \quad (42a)$$

and

$$Z(\tau_0,-u) = R(u) + \rho_s Z(\tau_0,u) + \rho_d G(u)\int_0^\infty Z(\tau_0,\mu)\mathrm{e}^{-\mu^2}\mu\,\mathrm{d}\mu \quad (42b)$$

for $u \in (0,\infty)$. Here, for the case of the finite slab, we have

$$Q(\tau) = \frac{\Delta}{u_0} c\pi^{-1/2}T(u_0)[\mathrm{e}^{-\tau/u_0} + \mathrm{e}^{-(\tau_0-\tau)/u_0}] \quad (43)$$

and

$$R(u) = (1-\Delta)2b\mathrm{e}^{-(b-1)u^2} + \rho_d G(u)T(u_0)\Delta\mathrm{e}^{-\tau_0/u_0} \ . \quad (44)$$

To conclude this section, we express the quantities we intend to compute, namely, the outgoing partial flux and the neutral distribution, as

$$O^* = T(u_0)\Delta\mathrm{e}^{-\tau_0/u_0} + \int_0^\infty Z(0,-u)\mathrm{e}^{-u^2}u\,\mathrm{d}u \quad (45)$$

and

$$\psi_*(\tau,u) = \mathrm{e}^{-u^2}Z(\tau,u) \ . \quad (46)$$

V. THE DISCRETE ORDINATES METHOD

The discrete ordinates solution we use in this work was developed in Ref. 5, and so we can make use of that material now to solve the half-space problems and the finite-slab problems that were defined in Sec. IV. We consider first the homogeneous version of Eq. (32), and so we approximate the integral term in Eq. (32) by a quadrature formula and write the homogeneous discrete ordinates equations to be solved as

$$u_i \frac{\mathrm{d}}{\mathrm{d}\tau} Z(\tau,u_i) + Z(\tau,u_i) = \sum_{k=1}^{N} w_k \Psi(u_k)[Z(\tau,u_k) + Z(\tau,-u_k)] \quad (47a)$$

and

$$-u_i \frac{\mathrm{d}}{\mathrm{d}\tau} Z(\tau,-u_i) + Z(\tau,-u_i) = \sum_{k=1}^{N} w_k \Psi(u_k)[Z(\tau,u_k) + Z(\tau,-u_k)] \quad (47b)$$

for $i = 1,2,\ldots,N$. In writing Eqs. (47), we have taken into account the fact that the characteristic function defined by Eq. (23) is an even function. In addition, we clearly are considering that the N quadrature points $\{u_k\}$ and the N weights $\{w_k\}$ are defined for use on the integration interval $[0,\infty)$. We note that it is to this feature of using a "half-range" quadrature scheme that we partially attribute the especially good accuracy we have obtained from the solution reported here.

Seeking exponential solutions, we substitute

$$Z(\tau,\pm u_i) = \phi(\nu,\pm u_i)\mathrm{e}^{-\tau/\nu} \quad (48)$$

into Eqs. (47) to find

$$\frac{1}{\nu}\boldsymbol{M}\boldsymbol{\Phi}_+ = (\boldsymbol{I}-\boldsymbol{W})\boldsymbol{\Phi}_+ - \boldsymbol{W}\boldsymbol{\Phi}_- \quad (49a)$$

and

$$-\frac{1}{\nu}\boldsymbol{M}\boldsymbol{\Phi}_- = (\boldsymbol{I}-\boldsymbol{W})\boldsymbol{\Phi}_- - \boldsymbol{W}\boldsymbol{\Phi}_+ \ , \quad (49b)$$

where $\boldsymbol{I}$ is the $N \times N$ identity matrix,

$$\boldsymbol{\Phi}_\pm = [\phi(\nu,\pm u_1),\phi(\nu,\pm u_2),\ldots,\phi(\nu,\pm u_N)]^T \ , \quad (50)$$

the superscript T denotes the transpose operation, the elements of the matrix $\boldsymbol{W}$ are

$$(\boldsymbol{W})_{i,j} = w_j\Psi(u_j) \quad (51)$$

and

$$\boldsymbol{M} = \mathrm{diag}\{u_1,u_2,\ldots,u_N\} \ . \quad (52)$$

If we now let

$$\boldsymbol{U} = \boldsymbol{\Phi}_+ + \boldsymbol{\Phi}_- \ , \quad (53)$$

then we can eliminate between the sum and the difference of Eqs. (49) to find

$$(\boldsymbol{D} - 2\boldsymbol{M}^{-1}\boldsymbol{W}\boldsymbol{M}^{-1})\boldsymbol{M}\boldsymbol{U} = \frac{1}{\nu^2}\boldsymbol{M}\boldsymbol{U} \ , \quad (54)$$

where

$$\boldsymbol{D} = \mathrm{diag}\{u_1^{-2},u_2^{-2},\ldots,u_N^{-2}\} \ . \quad (55)$$

Multiplying Eq. (54) by a diagonal matrix $\boldsymbol{T}$, we find

$$(\boldsymbol{D} - 2\boldsymbol{V})\boldsymbol{X} = \frac{1}{\nu^2}\boldsymbol{X} \ , \quad (56)$$

where

$$\boldsymbol{V} = \boldsymbol{M}^{-1}\boldsymbol{TWT}^{-1}\boldsymbol{M}^{-1} \tag{57}$$

and

$$\boldsymbol{X} = \boldsymbol{TMU} \ . \tag{58}$$

As discussed, for example, in Ref. 13, we can define the elements $T_1, T_2, \ldots, T_N$ of $\boldsymbol{T}$ so as to make $\boldsymbol{V}$ symmetric, and therefore, since $\boldsymbol{V}$ is a symmetric, rank one matrix, we can write our eigenvalue problem in the form

$$(\boldsymbol{D} - 2\boldsymbol{z}\boldsymbol{z}^T)\boldsymbol{X} = \lambda \boldsymbol{X} \ , \tag{59}$$

where $\lambda = 1/\nu^2$ and

$$\boldsymbol{z} = \left[\frac{\sqrt{w_1 \Psi(u_1)}}{u_1}, \frac{\sqrt{w_2 \Psi(u_2)}}{u_2}, \ldots, \frac{\sqrt{w_N \Psi(u_N)}}{u_N} \right]^T \ . \tag{60}$$

We note that the eigenvalue problem defined by Eq. (59) is of a form that is encountered when the so-called "divide-and-conquer" method[14] is used to find the eigenvalues of tridiagonal matrices. In addition, we see from Eq. (55) that, because of the way our basic eigenvalue problem is formulated, we must exclude zero from the set of quadrature points. Of course, to exclude zero from the quadrature set is not considered a serious restriction since typical Gauss quadrature schemes do not include the end points of the integration interval.

Considering that we have found the required eigenvalues from Eq. (59), we impose the normalization condition

$$\sum_{k=1}^{N} w_k \Psi(u_k)[\phi(\nu, u_k) + \phi(\nu, -u_k)] = 1 \ , \tag{61}$$

so that we can write our discrete ordinates solution of Eqs. (47) as

$$Z_h(\tau, \pm u_i) = \sum_{j=1}^{N} \left[A_j \frac{\nu_j}{\nu_j \mp u_i} \mathrm{e}^{-\tau/\nu_j} + B_j \frac{\nu_j}{\nu_j \pm u_i} \mathrm{e}^{-(\tau_0 - \tau)/\nu_j} \right] \ , \tag{62}$$

where the arbitrary constants $\{A_j\}$ and $\{B_j\}$ are to be determined from the boundary conditions, the separation constants $\{\nu_j\}$ are the reciprocals of the positive square roots of the eigenvalues defined by Eq. (59), and we have added the subscript h to remind us that Eq. (62) defines our discrete ordinates solution of the homogeneous version of Eq. (32).

It is clear from Eq. (62) that we cannot allow any separation constant to be equal to one of the quadrature points. We note that the constants $\{A_j\}$ and $\{B_j\}$ that are present in Eq. (62) will, as discussed in Sec. VI, be determined by fixing the behavior of $Z(\tau, u_i)$ at infinity (for half-space problems) and/or by constraining $Z(\tau, u_i)$ to meet discrete ordinates versions of the relevant boundary conditions.

Of course, Eqs. (32) and (41) are driven by inhomogeneous source terms, and so we now construct a particular solution to the inhomogeneous discrete ordinates equations

$$\pm u_i \frac{\mathrm{d}}{\mathrm{d}\tau} Z(\tau, \pm u_i) + Z(\tau, \pm u_i) = \sum_{k=1}^{N} w_k \Psi(u_k)[Z(\tau, u_k) + Z(\tau, -u_k)] + Q(\tau) \ , \tag{63}$$

where, in general, $Q(\tau)$ is given by Eq. (43). Now, seeking exponential solutions of Eq. (63), we obtain the particular solution

$$Z_p(\tau, \pm u_i) = \Gamma_0 T(u_0) \left[\frac{\mathrm{e}^{-\tau/u_0}}{u_0 \mp u_i} + \frac{\mathrm{e}^{-(\tau_0 - \tau)/u_0}}{u_0 \pm u_i} \right] \ , \tag{64}$$

where

$$\Gamma_0 = \frac{c\Delta}{\pi^{1/2}\Omega(u_0)} \tag{65}$$

and

$$\Omega(u_0) = 1 + 2u_0^2 \sum_{k=1}^{N} \frac{w_k \Psi(u_k)}{u_k^2 - u_0^2} \ . \tag{66}$$

We note that while the particular solution given by Eq. (64) has the merit of being simple, it must be used with caution since we cannot, without some algebraic reductions, allow $u_0 \in \{u_k\}$ and we cannot allow u_0 to be a zero of $\Omega(z)$ or, what is equivalent, $u_0 \in \{\nu_j\}$. A particular solution that does not require these restrictions is available in a recent paper[15] that reports a general procedure for constructing particular solutions for discrete ordinates approximations to quite general transport models.

Finally, we believe it is clear that a particular solution for the half-space case, that is, for a source term given by Eq. (34), is immediately available from Eq. (64) in the limit of infinite τ_0.

VI. SOLUTIONS TO THE PROBLEMS

Having developed our discrete ordinates formalism, we are now ready to solve the specific problems defined in Sec. IV.

VI.A. Half-Space Problems

For the half-space problems, we consider Eqs. (32) and (33a) and write

$$Z(\tau, \pm u_i) = \sum_{j=1}^{N} A_j \frac{\nu_j}{\nu_j \mp u_i} \mathrm{e}^{-\tau/\nu_j} + Z_p(\tau, \pm u_i) \ , \tag{67}$$

where

$$Z_p(\tau,\pm u_i) = \Gamma_0 \frac{e^{-\tau/u_0}}{u_0 \mp u_i} \tag{68}$$

and where the constants $\{A_j\}$ are to be determined. Now, substituting Eq. (67) into a discrete ordinates version of Eq. (33b), namely,

$$Z(0,u_i) - \rho_s Z(0,-u_i) - \rho_d G(u_i) \times \sum_{k=1}^{N} w_k u_k Z(0,-u_k) e^{-u_k^2} = R(u_i) \tag{69}$$

for $i = 1,2,\ldots,N$, we find a system of N linear algebraic equations we can solve to obtain the required $\{A_j\}$. And, so we can now write the desired solution as

$$O^* = \sum_{j=1}^{N} A_j \nu_j H(\nu_j) + O_p^* \ , \tag{70}$$

where

$$O_p^* = \Gamma_0 H(u_0) \tag{71}$$

and where, in general,

$$H(\pm\xi) = \sum_{k=1}^{N} \frac{w_k u_k}{\xi \pm u_k} e^{-u_k^2} \ . \tag{72}$$

VI.B. Finite-Slab Problems

Turning to the finite-slab problem, we note that the symmetry of the problem implies that

$$Z(\tau,u) = Z(\tau_0 - \tau, -u) \ , \tag{73}$$

and so we write

$$Z(\tau,\pm u_i) = \sum_{j=1}^{N} A_j \nu_j \left[\frac{e^{-\tau/\nu_j}}{\nu_j \mp u_i} + \frac{e^{-(\tau_0-\tau)/\nu_j}}{\nu_j \pm u_i} \right] + Z_p(\tau,\pm u_i) \ , \tag{74}$$

where now

$$Z_p(\tau,\pm u_i) = \Gamma_0 T(u_0) \left[\frac{e^{-\tau/u_0}}{u_0 \mp u_i} + \frac{e^{-(\tau_0-\tau)/u_0}}{u_0 \pm u_i} \right] \ . \tag{75}$$

In a manner analogous to that used for the half-space case, we determine the N required constants $\{A_j\}$ by substituting the solution given by Eq. (74) into the boundary condition [we choose to use Eq. (42a)] written as

$$Z(0,u_i) - \rho_s Z(0,-u_i) - \rho_d G(u_i) \times \sum_{k=1}^{N} w_k u_k Z(0,-u_k) e^{-u_k^2} = R(u_i) \tag{76}$$

for $i = 1,2,\ldots,N$. Once we have solved the system of linear algebraic equations so defined, we have the desired solution for the partial flux available from

$$O^* = O_p^* + T(u_0)\Delta e^{-\tau_0/u_0} + \sum_{j=1}^{N} A_j \nu_j [H(\nu_j) + H(-\nu_j) e^{-\tau_0/\nu_j}] \ , \tag{77}$$

where

$$O_p^* = \Gamma_0 T(u_0)[H(u_0) + H(-u_0) e^{-\tau_0/u_0}] \ . \tag{78}$$

In order to compute the neutral distribution $\psi_*(\tau,u)$, we first go back and substitute Eq. (74) into

$$u \frac{\partial}{\partial\tau} Z(\tau,u) + Z(\tau,u) = Q(\tau) + \sum_{k=1}^{N} w_k \Psi(u_k)[Z(\tau,u_k) + Z(\tau,-u_k)] \tag{79}$$

to obtain, after using the definition of the particular solution and the normalization condition given by Eq. (61),

$$u \frac{\partial}{\partial\tau} Z(\tau,u) + Z(\tau,u) = S_h(\tau) + S_p(\tau) \ , \tag{80}$$

where

$$S_h(\tau) = \sum_{j=1}^{N} A_j [e^{-\tau/\nu_j} + e^{-(\tau_0-\tau)/\nu_j}] \tag{81a}$$

and

$$S_p(\tau) = \frac{1}{u_0} \Gamma_0 T(u_0)[e^{-\tau/u_0} + e^{-(\tau_0-\tau)/u_0}] \ . \tag{81b}$$

Considering that the right side of Eq. (80) is known and keeping in mind the symmetry of the problem, we can solve that equation for $Z(\tau,u)$, $u \in [0,\infty)$, and use Eq. (46) to find our final result, namely,

$$\psi_*(\tau,u) = e^{-u^2}[\Upsilon(\tau,u) + \Xi_h(\tau,u) + \Xi_p(\tau,u)] \tag{82}$$

for $\tau \in [0,\tau_0]$ and $u \in [0,\infty)$. Here,

$$\Upsilon(\tau,u) = T(u)\{(1-\Delta)2b e^{-(b-1)u^2} + \rho_s[\Xi_h(\tau_0,u) + \Xi_p(\tau_0,u)] + \rho_d G(u) O^*\} e^{-\tau/u} \ , \tag{83}$$

where

$$\Xi_h(\tau,u) = \sum_{j=1}^{N} A_j \nu_j [C(\tau:\nu_j,u) + e^{-(\tau_0-\tau)/\nu_j} S(\tau:\nu_j,u)] \tag{84a}$$

and

$$\Xi_p(\tau,u) = \Gamma_0 T(u_0)[C(\tau:u_0,u) + \mathrm{e}^{-(\tau_0-\tau)/u_0} S(\tau:u_0,u)] \ . \tag{84b}$$

Finally, we note that the S and C functions we have used are defined by

$$S(z:x,y) = \frac{1-\mathrm{e}^{-z/x}\mathrm{e}^{-z/y}}{x+y} \tag{85a}$$

and

$$C(z:x,y) = \frac{\mathrm{e}^{-z/x}-\mathrm{e}^{-z/y}}{x-y} \ . \tag{85b}$$

VII. COMPUTATIONAL DETAILS AND RESULTS

Repeating some of the discussion given in previous works,[9–11] we note that what we must now do is to define the quadrature scheme to be used in our discrete ordinates solution. In this work, we used one of the (nonlinear) transformations

$$\xi(u) = \exp\{-u\} \tag{86a}$$

or

$$\xi(u) = \frac{1}{1+u} \tag{86b}$$

to map $u \in [0,\infty)$ into $\xi \in [0,1]$, and we then used the Gauss-Legendre scheme mapped (linearly) onto the interval $[0,1]$. Of course, other quadrature schemes could be used. In fact, we note that recent works by Garcia[16] and Gander and Karp[17] have reported special quadrature schemes for use in the general area of particle transport theory. Such an approach clearly could be used here. In fact, the choice of a quadrature scheme based on the integration interval $[0,\infty)$ with a weight function as defined by Eq. (23) seems a natural choice for this work. However, we have found the use of a mapping defined by either of Eqs. (86) followed by the use of the Gauss-Legendre integration formulas to be so effective that we have not developed any special-purpose quadrature schemes.

Continuing, we note that having defined our quadrature scheme and in developing a FORTRAN implementation of our solution, we found the required separation constants $\{\nu_j\}$ by using the special DZPACK numerical package[13] that was developed to take advantage of the special structure of Eq. (59) to solve the eigenvalue problem. The required separation constants were then available as the reciprocals of the square roots of these eigenvalues. We then used the subroutines DGECO and DGESL from the LINPACK package[18] to solve the relevant linear systems, and so, the solutions to the various problems were considered established.

Finally, but importantly, we note that since the function $\Psi(u)$ defined by Eq. (23) can be zero, from a computational point of view, we can have some, say, a total of N_0, of the separation constants $\{\nu_j\}$ effectively equal to some of the quadrature points $\{u_i\}$. Of course, this is not allowed in our discrete ordinates solution, and so, since the quadrature points where $\Psi(u_k)$ is effectively zero make no contribution to the right side of Eqs. (47), we have seen that we can simply omit these quadrature points from our calculation. Of course, in omitting these N_0 quadrature points, we have effectively changed N to $N - N_0$ in some aspects of our final solution. While this procedure can, we believe, be justified in terms of the numerics of the problem, a more elegant procedure, as was reported in Ref. 10, could have been used here.

In regard to numerical results, we must first note that the results listed (labeled as $c = 0.99$) in the last lines of the Tables 1 through 4 of Ref. 12 are not correct. Having reimplemented the F_N solution of Ref. 12 for half-spaces and slabs, we have discovered that these results were intended for $c = 0.999$, not $c = 0.99$, and that they are accurate only to two or three figures for the half-space cases and only to three or four figures for the slab cases.

In order to illustrate some of the merits of our developed discrete ordinates solutions to the considered problems, we list some typical results in Tables I and II for the half-space case and Tables III and IV for the case of finite slabs. We note that these numerical results are given with what we believe to be seven figures of accuracy. Of course, we have no proof of the accuracy of our results, but we have done various things to establish the confidence we have. First of all, we have increased the value of N used in our computations until we found stability in the final results, and we have also used numerical linear-algebra packages other than those mentioned and both nonlinear maps given by Eqs. (86) to obtain the same results as given in our tables. Moreover, when compared to converged results of the newly implemented version of the F_N method described in Ref. 12, our discrete ordinates results showed perfect agreement (seven figures of accuracy) for the half-space cases. In comparing our discrete ordinates results to new F_N results for the slab cases, we were able to confirm only five or six figures of accuracy since we were able to generate F_N results accurate only to five or six significant figures. We also have evaluated our result, as given by Eq. (82), for the neutral distribution, but since our results here are identical to those listed in Tables 5, 6, and 7 of Ref. 12, we do not list these results again.

We note that we have typically used $N = 50$ to generate the results listed in our tables, and to have an idea of the computational time required to solve a typical problem, we note that our FORTRAN implementation (no special effort was made to make the code especially efficient) of our discrete ordinates solution (with $N = 50$) runs in 0.1 s on a 400-MHz Pentium-based personal computer. Finally, to have some idea about N_0, the number of

TABLE I

The Partial Flux O^* for $\Delta = 1$, $u_0 = 20$, $a = 2$ and $\rho_d = 1 - \rho_s$

c	$\rho_s = 0.0$	$\rho_s = 0.2$	$\rho_s = 0.5$	$\rho_s = 0.8$	$\rho_s = 1.0$
0.1	1.504331(−3)	1.503308(−3)	1.501774(−3)	1.500239(−3)	1.499215(−3)
0.6	2.055885(−2)	2.043419(−2)	2.024713(−2)	2.005997(−2)	1.993512(−2)
0.9	1.231193(−1)	1.212665(−1)	1.185094(−1)	1.157781(−1)	1.139710(−1)
0.95	2.548871(−1)	2.500466(−1)	2.428879(−1)	2.358471(−1)	2.312164(−1)
0.99	1.178418	1.147835	1.103210	1.060008	1.031958
0.999	7.795792	7.553483	7.204017	6.870232	6.655851

TABLE II

The Partial Flux O^* for $\Delta = 0$, $b = 10$, $a = 2$ and $\rho_d = 1 - \rho_s$

c	$\rho_s = 0.0$	$\rho_s = 0.2$	$\rho_s = 0.5$	$\rho_s = 0.8$	$\rho_s = 1.0$
0.1	3.221114(−2)	3.220888(−2)	3.220550(−2)	3.220213(−2)	3.219989(−2)
0.6	3.302423(−1)	3.296144(−1)	3.286763(−1)	3.277427(−1)	3.271229(−1)
0.9	1.145045	1.134826	1.119652	1.104659	1.094761
0.95	1.789005	1.765409	1.730559	1.696341	1.673867
0.99	4.442183	4.344144	4.201159	4.062816	3.973035
0.999	1.470580(1)	1.427164(1)	1.364555(1)	1.304764(1)	1.266366(1)

TABLE III

The Partial Flux O^* for $\Delta = 1$, $u_0 = 20$, $a = 2$, $\rho_s = 0.2$ and $\rho_d = 0.5$

c	$\tau_0 = 1$	$\tau_0 = 2$	$\tau_0 = 5$	$\tau_0 = 10$	$\tau_0 = 20$
0.1	1.342815	1.160178	9.385386(−1)	7.013577(−1)	4.040951(−1)
0.6	1.668254	1.386900	1.084472	8.105791(−1)	4.742326(−1)
0.9	2.444931	2.066536	1.550503	1.145649	6.960800(−1)
0.95	2.785316	2.466757	1.916750	1.426124	8.866036(−1)
0.99	3.198505	3.087444	2.792396	2.357240	1.671273
0.999	3.319114	3.306183	3.265208	3.181403	2.955801

TABLE IV

The Partial Flux O^* for $\Delta = 0$, $b = 10$, $a = 2$, $\rho_s = 0.2$ and $\rho_d = 0.5$

c	$\tau_0 = 1$	$\tau_0 = 2$	$\tau_0 = 5$	$\tau_0 = 10$	$\tau_0 = 20$
0.1	1.053391(−1)	4.381968(−2)	3.246525(−2)	3.199429(−2)	3.197838(−2)
0.6	6.447509(−1)	4.199655(−1)	3.168462(−1)	3.061216(−1)	3.056348(−1)
0.9	1.903283	1.455076	1.018778	8.937392(−1)	8.762374(−1)
0.95	2.451692	2.050882	1.509680	1.262960	1.199360
0.99	3.116524	2.970013	2.642387	2.305978	2.035291
0.999	3.310470	3.293232	3.246483	3.174823	3.051371

quadrature points not included in some parts of our calculation, we note that using $\epsilon = 10^{-13}$ to decide if an eigenvalue and a quadrature point were the same "computationally," we found $N_0 = 2$ when $N = 50$ and the map defined by Eq. (86a) were used.

VIII. CONCLUDING REMARKS

In this work, we have successfully developed and implemented an analytical version of the discrete ordinates method for studying the transport of hydrogen atoms in a hydrogen plasma. And so, in addition to providing very high quality results for the considered problem, we have come to the conclusion that the techniques reported here, because of the very simple structure of the developed algorithm, can and (we expect) will be extended to analyze more realistic models[19] of the physical processes considered here.

Postscript: We would like to say here that we consider it an honor to be able to make a contribution to this issue of *Nuclear Science and Engineering* dedicated to the memory of G. C. Pomraning. While we had many wonderful exchanges with Jerry over the years, we are especially grateful to him for introducing us to the area of plasma physics we revisited in this current work. Of course, it was Jerry who, from basic physics, formulated for us the problems that we all went on to solve in our joint paper referred to in this work as Ref. 12. As all who knew him will testify, to collaborate and to develop research work with Jerry were enriching experiences that have made us all more able to see things clearly.

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