These are Appendixes to the paper by N. A. Almeida, M. S. Benilov, R. N. Franklin, and G. V. Naidis *Transition from a fully ionized plasma to an absorbing surface*, J. Phys. D: Appl. Phys. 37, No. 22, pp. 3107-3116 (2004).

APPENDIX A: ASYMPTOTIC BEHAVIOUR AT LARGE AND SMALL DISTANCES FROM THE EDGE OF THE SPACE-CHARGE SHEATH

Let us consider first the asymptotic behaviour of the solution to the problem (6)-(9) at large ξ. Following Ref. [15], we expand in $1-f$, w, and ν Eq. (6), Eq. (7), and Eq. (8) divided by $\delta^2\nu$. Retaining terms of the first order, one gets the equations

$$-\alpha\delta^2\frac{df}{d\xi}+\left(1+\alpha^2\right)w=0, \qquad \alpha\delta^2\frac{dw}{d\xi}=-\nu, \qquad \frac{\nu}{\delta^2}+f-1+\frac{w^2}{\nu}=0. \tag{A1}$$

Seeking a solution to these equations in an exponential form, one finds two one-parameter families of solutions that may be written as

$$\left\{\begin{array}{c} 1-f \\ w \\ \nu \end{array}\right\} = C_\pm \left\{\begin{array}{c} 1 \\ \mp\frac{\alpha\delta}{1+\alpha^2} \\ \frac{\alpha^2\delta^2}{1+\alpha^2} \end{array}\right\} \exp\left(\pm\frac{\xi}{\delta}\right), \tag{A2}$$

where C_+ and C_- are arbitrary constants. It should be emphasized that a linear combination of the two families is not a solution; in other words, if $C_+\neq 0$, then $C_-=0$ and *vice versa.* This situation, which is not typical for asymptotic behaviour of solutions of boundary-value problems, originates in the non-linearity of the last equation in Eq. (A1).

Solutions of the family involving the exponent with minus are compatible with the second boundary condition (9), solutions of the other family are not. Hence, one should set $C_+=0$.

Asymptotic behaviour of the solution to the problem (6)-(9) at small ξ, i.e., in the vicinity of the edge of the space-charge sheath, may be shown to be

$$w\left(\xi\right)=1+O\left(\sqrt{\xi}\right), \quad f\left(\xi\right)=f_w+O\left(\sqrt{\xi}\right), \tag{A3}$$

$$\nu\left(\xi\right)=\nu_w+O\left(\xi\right). \tag{A4}$$

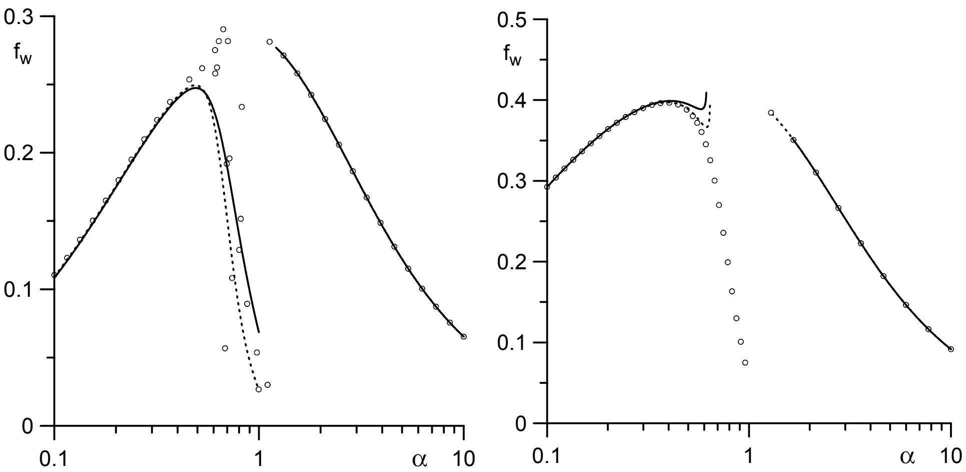
While the ion velocity and the number density show the square-root behaviour near the sheath edge which is characteristic for problems involving the Bohm criterion, this is not the case for the atomic number density.

APPENDIX B: STRAIGHTFORWARD NUMERICAL APPROACHES

A simple answer to the question which sign on the right-hand side of Eq. (20) is appropriate may be obtained as follows: on the basis of the requirement that Eq. (20) conform at small w to Eq. (16), one can assume that the proper sign is plus in the case $\alpha>1$ and minus in the case $\alpha<1$. Let us consider results of numerical calculations performed under this assumption. The calculations have been performed by means of the standard Runge-Kutta method of the fourth order (as well as all the other numerical calculations described in this work, unless otherwise is stated). The numerical grid was uniform (as well as in all the other numerical calculations described in this work) and contained 100 or 1000 steps, i.e., the step h was 10^{-2} or 10^{-3}. Calculations using the branch of ν with plus have been performed in the range $\alpha \geq 1$, calculations using the branch of ν with minus have been performed in the range $\alpha \leq 1$.

It has been found that negative values of the discriminant D occur and thus the calculations fail in a certain interval of α values around $\alpha = 1$. In the case $\beta = 1$, this interval includes only values above unity; note that at $\alpha = 1$ it is possible to obtain a solution with the use of the branch with minus but not of the branch with plus. With an increase of β the interval expands and includes values both below and above unity, as well as unity itself. The boundaries of this interval depend on h: the interval is narrower in calculations on a finer grid.

Results of successful calculations are shown in Fig. 7. One can see that the results are step-dependent in the range of α immediately below the above-mentioned interval. This is unusual given the fourth order of accuracy of the standard Runge-Kutta method being used.



(a) $\beta = 1$. (b) $\beta = 50$.

Figure 7. Results of straightforward numerical calculation of the dimensionless ion flux from the ionization layer. Lines: solution of the problem (14), (15) with the step $h = 10^{-2}$ (solid line) and with $h = 10^{-3}$ (dotted line). Points: solution of the problem (C2), (C3) with $h = 10^{-3}$.

In general, the above-described results do not provide a complete picture; in particular, they do not describe the range of α around the point of maximum of the dependence of f_w on α, which is of the most interest. Note that resorting to adaptive step size routines has not helped.

One could think that the difficulties arise due to the necessity to choose between different branches of the solution of the quadratic equation for the atomic density ν. On the other hand, if Eq. (8) is solved with respect to the charged-particle density f (rather than with respect to the atomic density ν), then there is only one positive solution and the problem of choosing between different branches does not arise. In order to make use of this fact, one should transform the second-order boundary-value problem (6), (7), (9) to a first-order initial-value problem for the function $\nu(w)$; see Appendix C below. The following numerical results have been obtained. For certain values of α, the calculations failed since negative values have occurred either of atomic density ν or of the charged-particle density f. In contrast to the calculations performed on the basis of Eq. (14), the values of α for which the calculations have failed do not constitute a continuous range (for example, for $\beta = 1$ with $h = 10^{-3}$ the calculations have failed at $\alpha = 0.688$ and $\alpha = 0.698$ but have been successful at $\alpha = 0.689$). Results of successful calculations are shown by points in Fig. 7 for some values of α and $h = 10^{-3}$. In the case $\beta = 1$, the calculation results are quite irregular for α around unity. For every β , the solution is step-dependent at α around unity. Thus this approach is unsatisfactory as well.

One could think that the above-described difficulties arise due to a failure of the method of Runge-Kutta, which is an explicit one; explicit methods are known to fail in certain situations (for example, in stiff problems, see, e.g., [1]). In this connection, calculations with the use of a second-order implicit method have been performed. At each knot of the numerical grid, an implicit finite-difference equation approximating Eq. (14) has been solved jointly with Eq. (8) by means of the Newton method. The results turned out to be similar to those described above and are equally unsatisfactory. Equally unsuccessful have been calculations in which a second-order implicit method was applied to Eq. (C2) instead of Eq. (14) [i.e., in which an implicit finite-difference equation approximating Eq. (14) has been solved at each knot of the numerical grid jointly with Eq. (8) by means of the Newton method].

APPENDIX C: DERIVING INITIAL-VALUE PROBLEM FOR THE FUNCTION $\nu(w)$

In order to transform the second-order boundary-value problem (6), (7), (9) to a first-order initial-value problem for the function $\nu(w)$, one can differentiate Eq. (8) with respect to ξ and then eliminate the derivatives $df/d\xi$ and $dw/d\xi$ by means of Eqs. (12) and (13). The resulting equation reads

$$\frac{d\nu}{d\xi} = -\frac{wf\nu\left[\alpha^2\nu + \left(\alpha^2 - 1\right)f\right]}{\alpha\left[2\nu - \delta^2\left(1 - f - w^2 f\right)\right]}. \tag{C1}$$

Dividing this equation by Eq. (13), one obtains

$$\frac{d\nu}{dw} = \frac{\delta^2 wf\nu\left(1 - w^2\right)\left[\alpha^2\nu + \left(\alpha^2 - 1\right)f\right]}{\left[\nu + w^2\left(1 + \alpha^2\right)(\nu + f)\right]\left[2\nu - \delta^2\left(1 - fw^2 - f\right)\right]}. \tag{C2}$$

This equation is supplemented by the expression for the charged-particle density obtained by solving Eq. (8) with respect to f. There is only one positive solution and the problem of choosing between different branches does not arise.

Eq. (C2) should be solved for the function $\nu(w)$ on the interval $0 \le w \le 1$ with the initial condition

$$\nu(0) = 0. \tag{C3}$$

The right-hand side of Eq. (C2) at $w = 0$ should be evaluated by means of the second equation in Eq. (16) with the lower sign in order to avoid uncertainty.

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[1] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in FORTRAN*, 2nd ed., Cambridge University Press, Cambridge, 1992

APPENDIX D: ASYMPTOTIC BEHAVIOUR OF THE FUNCTION $f(w)$ IN THE VICINITY OF THE LINE Γ

This behaviour is sought in the form of an expansion

$$f(w) = f_\Gamma + C_3\varepsilon + C_4\varepsilon^2 + \ldots, \tag{D1}$$

where $\varepsilon = w - w_\Gamma$. Substituting this expansion into Eq. (14), expanding in ε and retaining terms of the order unity, one finds

$$C_3 = -\frac{2\delta^3\alpha^6}{\left(\alpha^4\beta+1\right)^2}. \tag{D2}$$

Asymptotic behaviour of the function $\nu(w)$ in the vicinity of the boundary should be found in order to determine C_4. To this end, we expand Eq. (18) and the first term on the right-hand side of Eq. (20):

$$D = \frac{1-\alpha^2}{\alpha^2}\left(R_1 - C_4\right)\varepsilon^2 + O\left(\varepsilon^3\right), \tag{D3}$$

$$\frac{\delta^2}{2}\left(1 - f - w^2 f\right) = \nu_\Gamma + \frac{\delta^3\alpha^4\left(\alpha^4\beta + 2\alpha^2 - 1\right)}{\left(\alpha^4\beta+1\right)^2}\varepsilon + O\left(\varepsilon^2\right), \tag{D4}$$

where

$$R_1 = \frac{\delta^4\alpha^8\left(3-\alpha^4\beta\right)}{\left(\alpha^4\beta+1\right)^3}. \tag{D5}$$

Substituting Eqs. (D3) and (D4) into Eq. (20), one finds

$$\nu = \nu_\Gamma + \frac{\delta^3\alpha^4\left(\alpha^4\beta + 2\alpha^2 - 1\right)}{\left(\alpha^4\beta+1\right)^2}\varepsilon + \frac{\delta\left(1-\alpha^2\right)^{1/2}\left(R_1 - C_4\right)^{1/2}}{\alpha}\varepsilon + O\left(\varepsilon^2\right). \tag{D6}$$

Note that the third term on the right-hand side of this equation has been written with account of the fact that the range of α being considered is below unity and that the branch with minus should be chosen in Eq. (20) at $w < w_\Gamma$ and the branch with plus at $w > w_\Gamma$.

Substituting Eqs. (D1) and (D6) into Eq. (14), expanding in ε and equating terms of the order of ε, one arrives at the following equation governing constant C_4:

$$2C_4 = -R_2 + R_3\left(R_1 - C_4\right)^{1/2}, \tag{D7}$$

where

$$R_2 = \frac{\delta^4\alpha^8\left(\alpha^6\beta + 2\alpha^4\delta^2 - \alpha^2 - 6\right)}{\left(\alpha^4\beta+1\right)^3}, \tag{D8}$$

$$R_3 = \frac{\delta^2\left(\delta+1\right)\alpha^5\left(\alpha^2+1\right)\left(\alpha^2\delta - \alpha^2 + 1\right)\left(\alpha^2 - \alpha_{cr}^2\right)}{\left(\alpha^4\beta+1\right)^2\left(1-\alpha^2\right)^{1/2}}. \tag{D9}$$

It is convenient to rewrite Eq. (D7) as a quadratic equation for $\left(R_1 - C_4\right)^{1/2}$

$$2\left(R_1 - C_4\right) + R_3\left(R_1 - C_4\right)^{1/2} - \left(2R_1 + R_2\right) = 0. \tag{D10}$$

Note that

$$2R_1 + R_2 = \frac{\delta^4 (\delta+1) \alpha^{10} (\alpha^2\delta - \alpha^2 + 1)(\alpha^2 - \alpha_{cr}^2)}{(\alpha^4\beta + 1)^3}. \tag{D11}$$

Discriminant of Eq. (D10), $R_4 = R_3^2 + 16R_1 + 8R_2$, may be evaluated to be

$$R_4 = \alpha^{10}\delta^4 (\delta+1) \left(\alpha^2\delta - \alpha^2 + 1\right) \left(\alpha^2 - \alpha_{cr}^2\right) \times \frac{(3-\alpha^2)^2 \alpha^4\delta^2 + (7-\alpha^2)(\alpha^2+1)(1-\alpha^2)^2}{(\alpha^4\beta+1)^4 (1-\alpha^2)}. \tag{D12}$$

One can see that $R_4 > 0$ in the range $\alpha_{cr} < \alpha < 1$ and Eq. (D10) is solvable. Since $2R_1 + R_2 > 0$ in this range, one of the roots of this equation is positive and the other is negative, the positive root being

$$(R_1 - C_4)^{1/2} = \frac{\sqrt{R_4} - R_3}{4}. \tag{D13}$$

Thus, a smooth switching between the two branches of the solution is possible. It is of interest to note that, while being possible in the range $\alpha_{cr} < \alpha < 1$, it would not be possible in the range $\alpha < \alpha_{cr}$, where $R_4 < 0$ and Eq. (D10) turns unsolvable.

APPENDIX E: ASYMPTOTIC BEHAVIOUR OF THE FUNCTION $f(w)$ AT SMALL w

Let us first consider a particular solution to the problem (14), (15), (8) with the asymptotic behaviour at small w represented by a power series,

$$f = \sum_{n=0}^{\infty} p_n w^n. \tag{E1}$$

We need to find the coefficients $p_0, p_1, p_2, \ldots$. It follows from Eq. (15) and the first equation in Eq. (16) that

$$p_0 = 1, \quad p_1 = -\frac{1+\alpha^2}{\alpha\delta}. \tag{E2}$$

The next coefficients may be found by substituting expansion (E1) into Eqs. (14), (8) and expanding. In particular,

$$p_2 = \left(\frac{1+\alpha^2}{\alpha\delta}\right)^2 - \frac{\alpha^4 + 2\alpha^2 - 1}{3\alpha^2 - 1}, \tag{E3}$$

$$p_3 = -\left(\frac{1+\alpha^2}{\alpha\delta}\right)^3 - \frac{(1+\alpha^2)\left[\alpha^8\delta^2 - (9\alpha^6 + 10\alpha^4 - 15\alpha^2 + 4)(3\alpha^2 - 1)\right]}{2\alpha\delta (3\alpha^2-1)^2 (2\alpha^2 - 1)}. \tag{E4}$$

Expressions for the following coefficients are involved; we write down here only the denominator of the fraction part of the expression for p_4:

$$(\alpha\delta)^4 \left(3\alpha^2 - 1\right)^3 \left(2\alpha^2 - 1\right) \left(5\alpha^2 - 3\right). \tag{E5}$$

Note that coefficients p_2, p_3, p_4 and, presumably, all the following have singularities at $\alpha^2 = 1/3$; coefficients p_3, p_4 and, presumably, all the following have singularities at $\alpha^2 = 1/2$; coefficient p_4 and, presumably, all the following have singularities at $\alpha^2 = 3/5$; *etc.* One should expect therefore that Eq. (14) has at $\alpha^2 = \frac{1}{3}, \frac{1}{2}, \frac{3}{5}, \ldots$ no solutions with the asymptotic behaviour at small w in the form of a power series (E1).

Proceed to finding the asymptotic behaviour of a general solution of Eq. (14). This behaviour is sought in the form

$$f = 1 + p_1 w + \gamma, \tag{E6}$$

where $\gamma = \gamma(w)$ is an unknown function which tends at $w \to 0$ to zero faster than w but slower than w^2.

Asymptotic behaviour of the function $\nu(w)$ may be found by substituting Eq. (E6) into Eq. (8). One finds

$$\nu = \alpha\delta w - \frac{\alpha^2\delta^2}{\alpha^2 - 1}\gamma + \ldots. \tag{E7}$$

Substituting Eqs. (E6) and (E7) into Eq. (14) and expanding, one arrives at an equation for function γ

$$w\frac{d\gamma}{dw} = \frac{1+\alpha^2}{1-\alpha^2}\gamma. \tag{E8}$$

A (general) solution to this equation reads

$$\gamma = C_1\, w^{\left(1+\alpha^2\right)/\left(1-\alpha^2\right)}, \tag{E9}$$

where C_1 is an arbitrary constant. One can see that the assumption that γ tends at $w \to 0$ to zero faster than w but slower than w^2 holds in the range $0 < \alpha^2 < 1/3$. Thus, the derivation applies in the range $0 < \alpha^2 < 1/3$ and the asymptotic behaviour of a general solution to Eq. (14) at small w for such α is

$$f = 1 + p_1 w + C_1\, w^{\left(1+\alpha^2\right)/\left(1-\alpha^2\right)} + \ldots. \tag{E10}$$

The asymptotic behaviour of a general solution of Eq. (14) in the vicinity of the point $w = 0$, applicable at bigger values of α, is sought in the form

$$f = 1 + p_1 w + p_2 w^2 + \gamma, \tag{E11}$$

where $\gamma = \gamma(w)$ is an unknown function which tends at $w \to 0$ to zero faster than w^2 but slower than w^3. Eq. (E7) is replaced by

$$\nu = \alpha\delta w + \frac{\alpha^4\delta^2 - 3\alpha^4 - 2\alpha^2 + 1}{3\alpha^2 - 1}w^2 - \frac{\alpha^2\delta^2}{\alpha^2 - 1}\gamma + \ldots, \tag{E12}$$

Eqs. (E8) and (E9) remain applicable. One can conclude that the assumption that γ tends at $w \to 0$ to zero faster than w^2 but slower than w^3 holds in the range $1/3 < \alpha^2 < 1/2$ and the asymptotic behaviour of a general solution to Eq. (14) at small w is for such α

$$f = 1 + p_1 w + p_2 w^2 + C_1\, w^{\left(1+\alpha^2\right)/\left(1-\alpha^2\right)} + \ldots. \tag{E13}$$

It is legitimate to assume that the asymptotic behaviour applicable at any positive α below unity may be written in the form of Eq. (28). For simplicity, we do not consider cases $\alpha^2 = (m-1)/(m+1)$ $(m = 2, 3, 4, \dots)$, where the coefficient p_m and all the following become infinite [and $(1+\alpha^2)/(1-\alpha^2)$ becomes equal to m, i.e., takes a natural value].

One can see from Eq. (28) that in the case $0 < \alpha < 1$ the general solution to Eq. (14) represents a one-parameter family of solutions, each of them satisfying the boundary condition $f(0) = 1$. In other words, in the case $0 < \alpha < 1$ this boundary condition does not allow one to choose between different solutions, i.e., is ineffective, and the initial-value problem for the function $f(w)$, comprised by Eqs. (14), (8) and by the boundary condition (15), has multiple solutions (i.e., is not closed).

The present analysis has not revealed multiplicity of solutions in the case $\alpha = 0$. (Note that this conclusion conforms to the analysis of Ref. [15], in which a unique asymptotic solution has been found in the limiting case $\alpha \to 0$.) Therefore one should assume that $C_1 \to 0$ as $\alpha \to 0$ or, in other words, that different solutions of the initial-value problem tend to a single solution as α tends to zero.

APPENDIX F: ASYMPTOTIC BEHAVIOUR OF EXPONENTIALLY DECAYING SOLUTIONS TO THE BOUNDARY-VALUE PROBLEM

The choice between the upper and lower signs in Eq. (16) represents in the framework of the initial-value problem an analogue of the choice between exponentially growing and exponentially decaying solutions in the boundary-value problem. The choice of the lower sign in Eq. (16), which resulted in a negative p_1 in the treatment of Appendix E, corresponds to the choice of exponentially decaying solutions in the framework of the boundary-value problem. Since there is a one-parameter family of solutions with negative p_1 to Eq. (14) in the case $0 < \alpha < 1$ (rather than a unique solution), one should expect that exponentially decaying solutions to the boundary-value problem represent in the case $0 < \alpha < 1$ a two-parameter (rather than a one-parameter) family.

Let us prove that the latter is indeed the case. We seek asymptotic behaviour of exponentially decaying solutions to the boundary-value problem in the form

$$\left\{ \begin{array}{c} 1-f \\ w \\ \nu \end{array} \right\} = C_- \left\{ \begin{array}{c} 1 \\ \frac{\alpha\delta}{1+\alpha^2} \\ \frac{\alpha^2\delta^2}{1+\alpha^2} \end{array} \right\} \exp\left(-\frac{\xi}{\delta}\right) + \left\{ \begin{array}{c} C_5 \\ \frac{\alpha\delta}{1+\alpha^2} C_6 \\ \frac{\alpha^2\delta^2}{1+\alpha^2} C_7 \end{array} \right\} \exp\left(-s\frac{\xi}{\delta}\right), \tag{F1}$$

where C_- is an arbitrary constant and C_5, C_6, C_7, and s are constants that, in principle, need to be determined, $1 < s < 2$. Substituting these expressions into Eq. (6), Eq. (7), and Eq. (8) divided by $\delta^2\nu$, expanding and retaining terms of the order of $\exp(-s\xi/\delta)$, one gets

$$C_5 = \frac{C_6}{s}, \quad C_7 = C_6 s, \quad s = \frac{1+\alpha^2}{1-\alpha^2}. \tag{F2}$$

One can see that the assumption that $1 < s < 2$ holds in the range $0 < \alpha^2 < 1/3$. Thus, the derivation applies in the range $0 < \alpha^2 < 1/3$ and so does the asymptotic behaviour (F1). It is legitimate to assume that the asymptotic behaviour at any positive α below unity may be written in a form similar to Eq. (28):

$$\left\{ \begin{array}{c} 1-f \\ w \\ \nu \end{array} \right\} = C_{-} \left\{ \begin{array}{c} 1 \\ \frac{\alpha\delta}{1+\alpha^2} \\ \frac{\alpha^2\delta^2}{1+\alpha^2} \end{array} \right\} \sum_{n=1}^{\infty} q_n \exp\left(-n\frac{\xi}{\delta}\right) + C_6 \left\{ \begin{array}{c} \frac{1-\alpha^2}{1+\alpha^2} \\ \frac{\alpha\delta}{1+\alpha^2} \\ \frac{\alpha^2\delta^2}{1-\alpha^2} \end{array} \right\} \left[\exp\left(-\frac{1+\alpha^2}{1-\alpha^2}\frac{\xi}{\delta}\right) + \dots\right], \tag{F3}$$

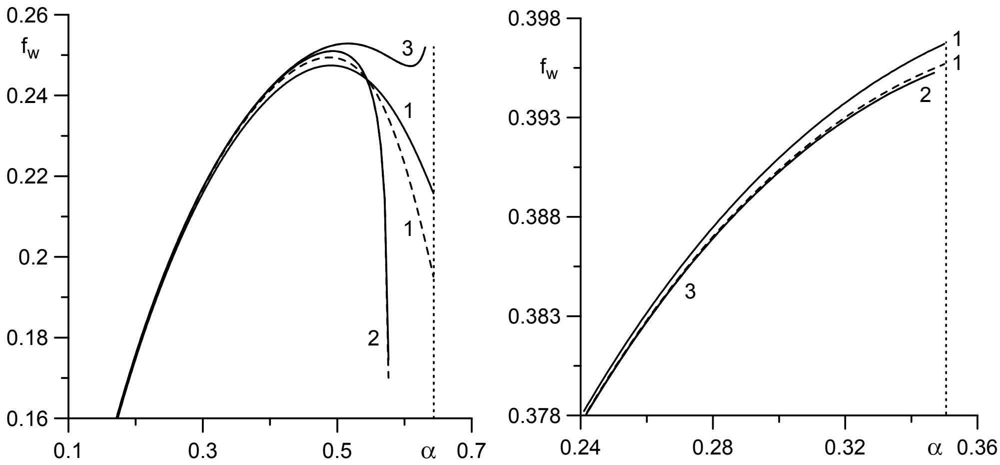
where $q_1 = 1$ and q_n $(n = 2, 3, \dots)$ are coefficients depending on α and δ.

It follows from Eq. (F3) that the family of exponentially decaying solutions to the boundary-value problem in the case $0 < \alpha < 1$ is governed by two parameters, C_{-} and C_6. Since one boundary condition, the first equation in Eq. (9), is in a general case insufficient to determine two free parameters, this means that the boundary-value problem in the case $0 < \alpha < 1$ is not closed.

In other words, we have shown that although the boundary condition $f|_{\xi\to\infty} = 1$ does allow one to eliminate exponentially growing solutions of the original boundary-value problem, exponentially decaying solutions in the case $0 < \alpha < 1$ are governed by two (rather than one) arbitrary constants and the boundary-value problem is not closed, as is the initial-value problem for the function $f(w)$.

APPENDIX G: ADDITIONAL NUMERICAL VERIFICATION OF ANALYTICAL RESULTS

Eq. (28) shows that in the case $0 < \alpha < 1$ the asymptotic behaviour at small w of solutions of Eq. (14) [supplemented with Eq. (20) with minus] includes, in addition to natural powers of w [the first term on the right-hand side of Eq. (28)], also fractional powers (the second term). In other words, solutions are not infinitely differentiable at $w = 0$. This may cause a decrease of the actual accuracy of the (standard fourth-order) Runge-Kutta method and render results step-dependent. The latter is confirmed by the results of numerical solution of Eq. (14) [supplemented with Eq. (20) with minus] with initial condition (15) shown in Fig. 7. (Part of these results is reproduced on a larger scale in Fig. 8; lines 1).



(a) $\beta = 1$.

(b) $\beta = 50$.

Figure 8. Dimensionless ion flux from the ionization layer for $\alpha < \alpha_{cr}$. Solid: 100 steps. Dashed: 1000 steps. Dotted: the value $\alpha = \alpha_{cr}$. 1: solution of the problem (14), (15). 2: particular solution to Eq. (14) which is infinitely differentiable at $w = 0$. 3: solution of the boundary-value problem.

It was shown in Appendix E that $C_1 \to 0$ as $\alpha \to 0$, meaning that the second term on the right-hand side of Eq. (28), which contains fractional powers, vanishes at small α. Hence, numerical results for the function $f(w)$ must turn step-independent as α decreases. One can see from Figs. 7 and 8 that this is indeed the case.

It follows from the analytical treatment that Eq. (14) in the case $0 < \alpha < 1$ has a particular solution which is infinitely differentiable at $w = 0$, namely the one described by Eq. (28) with $C_1 = 0$. This conclusion may be numerically verified as follows (for simplicity, we consider only the range $\alpha \leq \alpha_{cr}$). At $\alpha = \alpha_{cr}$, the second term on the right-hand side of Eq. (28) is at $w \to 0$ of the order $w^{1+2/\delta}$. It follows that this term is at $\alpha \leq \alpha_{cr}$ greater than or equal to w^3. Therefore, the condition

$$f = 1 + p_1 w + p_2 w^2 + p_3 w^3 + o\left(w^3\right) \tag{G1}$$

ensures at $\alpha \leq \alpha_{cr}$ that the second term on the right-hand side of Eq. (28) is eliminated and the function $f(w)$ is infinitely differentiable at $w = 0$. The condition (G1) can be implemented by transforming the problem to the new unknown function

$$z(w) = \frac{f - (1 + p_1 w + p_2 w^2)}{w^3}, \tag{G2}$$

for which the condition (G1) assumes the simple form $z(0) = p_3$. Results of calculations performed with the use of this approach are depicted by lines 2 in Fig. 8. The results of solution with $h = 10^{-2}$ and $h = 10^{-3}$ can hardly be distinguished, as it was expected.

It was shown in Appendix F that the original boundary-value problem, represented by Eqs. (6), (7), (9), at $0 < \alpha < 1$ is not closed, i.e., has multiple solutions, as does the initial-value problem for the function $f(w)$. However, these solutions are infinitely differentiable, in contrast to solutions of the initial-value problem (which are not infinitely differentiable at $w = 0$). Hence, results obtained by solving the original boundary-value problem should be step-independent. In order to verify this conclusion, the boundary-value problem (6), (7), (9) has been solved numerically as follows. Eq. (12) may be rewritten as

$$w = \frac{\alpha\delta^2 \left(1 - w^2\right)}{f \left[\nu + \left(1 + \alpha^2\right)(\nu + f)\right]} \frac{df}{d\xi}. \tag{G3}$$

Substituting this expression into Eq. (7), one arrives at a second-order equation for the function f:

$$\alpha^2\delta^4 \frac{d}{d\xi} \left[\frac{1 - w^2}{\nu + \left(1 + \alpha^2\right)(\nu + f)} \frac{df}{d\xi} \right] = -f\nu, \tag{G4}$$

This equation has a singularity at $\xi = 0$, which is related to the square-root behaviour of the ion velocity and the number density near the sheath edge, described by Eq. (A3). In order to remove the singularity, one can introduce a new independent variable

$$\eta = \int_0^\xi \frac{d\xi}{1 - w^2}. \tag{G5}$$

One gets the boundary-value problem

$$\alpha^2\delta^4 \frac{d}{d\eta} \left[\frac{1}{\nu + \left(1 + \alpha^2\right)(\nu + f)} \frac{df}{d\eta} \right] = -\nu \left(1 - w^2\right) f, \tag{G6}$$

$$\eta = 0: \qquad \alpha\delta^2 \frac{df}{d\eta} - f \left[\nu + \left(1 + \alpha^2\right)(\nu + f)\right] = 0, \tag{G7}$$

$$f(\infty) = 1, \tag{G8}$$

where w is related to f by the equation

$$w = \frac{\alpha\delta^2}{f \left[\nu + \left(1 + \alpha^2\right)(\nu + f)\right]} \frac{df}{d\eta}. \tag{G9}$$

Since we are interested in solving this problem primarily in the range $\alpha < \alpha_{cr}$, the branch of function ν with minus should be chosen and one can write

$$\nu = \frac{\delta}{F_1} f w, \tag{G10}$$

where

$$F_1 = \frac{\delta}{2} \left(\frac{1 - f}{wf} - w \right) + \left[\frac{\delta^2}{4} \left(\frac{1 - f}{wf} - w \right)^2 - 1 \right]^{1/2}. \tag{G11}$$

Making use of Eq. (G9), one can rewrite Eq. (G6) as

$$\alpha^2\delta^4 \frac{d}{d\eta} \left(F_2 \frac{df}{d\eta} \right) = F_3 f \frac{df}{d\eta}, \tag{G12}$$

where

$$F_2 = \frac{1}{\nu + \left(1 + \alpha^2\right)(\nu + f)}, \quad F_3 = -\frac{\alpha\delta^3 \left(1 - w^2\right)}{F_1 \left[\nu + \left(1 + \alpha^2\right)(\nu + f)\right]}, \tag{G13}$$

and ν is given by Eq. (G10).

In calculations, the boundary condition (G8) is applied at $\eta = \eta_{\max}$, where $\eta_{\max}$ is a certain value of η which is finite but large enough. It is convenient to replace this condition by the following boundary condition at $\eta = \eta_{\max}$, which follows from the asymptotic behaviour (A2):

$$\delta \frac{df}{d\eta} + f - 1 = 0. \tag{G14}$$

The condition (G14) is applicable at lower $\eta_{\max}$ than the condition (G8), which allows one to reduce the interval of numerical calculations.

The boundary-value problem (G12), (G7), (G14) is solved numerically by iterations. Coefficients F_2 and F_3 and the quantity in the square brackets in Eq. (G7) are calculated in terms of the previous iteration, the product $f\, df/d\eta$ is linearized by means of the Newton method. The linearized problem is solved using the Petukhov method[2], which is a method for solving linear boundary-value problems based on a fourth-order finite-difference scheme. For each δ, calculations started from a small value of α, the initial approximation being as follows:

$$f = \frac{f_w}{f_w + (1 - f_w)\, e^{-\eta/\delta}}, \quad f_w = \frac{\alpha\delta}{\alpha\delta + 1}, \tag{G15}$$

$$\nu = (\alpha\delta)^2 \, (1 - f)\,. \tag{G16}$$

(These formulas may be derived from the asymptotic solution for small α, Ref. [15].) The calculations proceeded with gradually increasing α, the solution obtained for a current value of α being used as an initial approximation for the subsequent value. The iterations have been found to fail to converge when α approached α_{cr}.

Results of calculations performed with the use of this approach are depicted in Fig. 8 by lines 3. Results obtained with 100 and 1000 steps (for the same interval of numerical integration) cannot be distinguished on the graph, as it was expected.

Various solutions shown in Fig. 8a manifest an appreciable difference only in the range $0.4 \lesssim \alpha \leq \alpha_{cr}$. This result may be understood in view of the conclusion of Appendix E that different solutions become close between themselves as α tends to zero. As β increases, α_{cr} decreases and difference between various solutions in the range $\alpha < \alpha_{cr}$ should decrease. This tendency indeed is present in the numerical results: solutions shown in Fig. 8b differ between themselves by no more than a few per cent in the whole range $\alpha < \alpha_{cr}$.

APPENDIX H: TRANSITION OF THE ATOMIC FLOW THROUGH THE SOUND BARRIER

The line Γ has appeared in the analysis of Sec. 3.1, which is based on solving a problem for the function f supplemented with the quadratic equation for ν, as a boundary

[2] I. V. Petukhov, in *Methods of Numerical Solution of Differential and Integral Equations and Quadrature Formulas (Supplement to Journal of Computational Mathematics and Mathematical Physics)*, (Nauka, Moscow, 1964), pp. 304–325.

separating the calculation domain into parts in which different branches of solution for ν are appropriate. A question arises whether this line would appear in the framework of an approach based on solving a problem for the function ν supplemented with the quadratic equation for f; we remind that there is no switching between different branches in the framework of this approach. This question is considered here.

Let us introduce the sound velocity of the atomic fluid, $u_a = \sqrt{kT_h/m_i}$, and the normalized velocity (the Mach number) of the flow of the atomic fluid, $w_a = v_a/u_a$. It follows from the second equation in Eq. (1) that $w_a = \delta f w/\nu$. Making use of Eq. (A2), one finds $w_a|_{\xi\to\infty} = 1/\alpha$. Hence, the atoms leave the ionization layer for the bulk plasma with a sub-sonic velocity if α is above unity and with a super-sonic velocity if α is below unity.

Transforming the denominator of Eq. (C1) with the use of Eq. (8), one can write

$$\frac{d\nu}{d\xi} = -\frac{wf\left[\alpha^2\nu + \left(\alpha^2 - 1\right)f\right]}{\alpha\left(1 - w_a^2\right)}. \tag{H1}$$

The denominator of the right-hand side of this equation is proportional to $(1 - w_a^2)$ as it should have been expected; cf. Eq. (12). Hence, the denominator of the right-hand side of Eq. (H1) vanishes at the sound barrier. If the transition of the atomic flow through the sound barrier occurs inside the ionization layer, the numerator of the right-hand side of Eq. (H1) must vanish at the barrier, otherwise the derivative $d\nu/d\xi$ would be infinite and the transition would not be smooth. It should be emphasized that the numerator of the right-hand side of Eq. (H1) in principle may vanish, in contrast to the numerator of the corresponding equation for the ion fluid, Eq. (12), which is always positive and as a consequence the ion flow reaches the ion sound barrier at the sheath edge, i.e., at a boundary of the ionization layer rather than inside it.

Writing the condition $w_a = 1$ in the form

$$\nu = \delta f w \tag{H2}$$

and solving the latter equation jointly with the condition of vanishing numerator of the right-hand side of Eq. (H1),

$$\alpha^2\nu = \left(1 - \alpha^2\right) f, \tag{H3}$$

and with Eq. (8), one arrives at Eqs. (25) and (26), describing the line Γ. Thus, the atomic flow crosses the sound barrier inside the ionization layer in the case $\alpha_{cr} < \alpha < 1$ and this transition occurs on the line Γ. Taking into account that $w_a|_{\xi\to\infty} = 1/\alpha > 1$ at $\alpha < 1$, one should assume that the atomic flux is sub-sonic before the barrier (at $w > w_\Gamma$) and super-sonic after the barrier (at $w < w_\Gamma$). In the case $\alpha \geq 1$, the atomic flow does not cross the sound barrier and remains sub-sonic throughout the ionization layer. In the case $\alpha \leq \alpha_{cr}$, the atomic flow is super-sonic throughout the layer.

One can conclude that if the atomic flow at a given point in space and given values of α and δ is sub-sonic (super-sonic), then the appropriate branch of the expression for ν, Eq. (20), is the one with plus (minus). The correctness of this conclusion can be seen also from Eq. (8): product of the two roots of this equation equals $(\delta w f)^2$, hence the bigger root (the one with plus) exceeds $\delta w f$ (which amounts to $w_a < 1$) while the smaller root is below $\delta w f$ (which amounts to $w_a > 1$).

Thus, the answer to the question formulated at the beginning of this Appendix is positive: the line Γ appears in a natural way not only when a problem for f is treated, but also when a problem for ν is treated. In the latter context, Γ may be considered as the Mach line, i.e., a boundary dividing the strip $(0 < \alpha < \infty,\ 0 \leq w \leq 1)$ into parts in which the atomic flow inside the ionization layer is sub- or super-sonic.

APPENDIX I: INTERPOLATION FORMULA FOR THE ION FLUX

Asymptotic behaviour of the function $f_w(\alpha, \delta)$ in the limiting cases $\alpha \to 0$ and $\alpha \to \infty$ was calculated in Ref. [15] and reads, respectively,

$$f_w(\alpha, \delta) \approx \delta\alpha - 2\delta^2\alpha^2, \tag{I1}$$

$$f_w(\alpha, \delta) \approx \frac{C_2}{\alpha}, \tag{I2}$$

where

$$C_2 = \frac{\delta \left(\delta^4 - 1 - 4\delta^2 \ln\delta\right)^{1/2}}{\left(\delta^2 - 1\right)^{3/2}}. \tag{I3}$$

Eq. (50) of Ref. [15] represents a rational fraction in α with coefficients determined with the use of Eqs. (I1) and (I2). One can try to obtain a more accurate approximation by making use, in addition to the asymptotic behaviours of $f_w(\alpha)$ at small and large α, also of the fact that $\alpha = \alpha_{cr}$ is a point of maximum of $f_w(\alpha)$. The simplest formula of this kind reads

$$f_w = \frac{\delta C_2\sqrt{1+\delta}\alpha}{C_2\sqrt{\delta+1} + \left[C_2\left(2\sqrt{\delta+1}-1\right)(\delta+1) - \delta\right]\alpha + \delta\sqrt{1+\delta}\alpha^2}. \tag{I4}$$

This formula satisfies the condition $f_w(\alpha_{cr}) = \delta/2\,(1+\delta)$ and conforms in the limiting cases $\alpha \to 0$ and $\alpha \to \infty$ to the first approximation of Eq. (I1) and to Eq. (I2), respectively.

Note that one is tempted to derive a still more accurate approximate formula by taking into account the second approximation in Eq. (I1) and the equality $df_w/d\alpha\,(\alpha_{cr}) = 0$. However, this attempt turns out unsuccessful: such a formula has a singularity (at a certain value of α below unity) for some values of β.