Multi-term approach to angle dependence in the Boltzmann distribution function

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Abstract: In overwhelming majority of works on plasma physics the electron distribution function is used in so named two-term Lorentz approximation for velocity directions. It is caused by large dimension of phase space, in which a distribution function is to be appeared, and a search for simplification. In many of situations the function is almost isotropic indeed. But there exist also situations, where this approximation is not sufficient. Simplest of them – an absorbing wall – is considered here.

Keywords: Absorbing wall, electron distribution function, low angle scattering, Legendre polynomial expansion.

1. Introduction

The Boltzmann equation in its generalized form is a source of many creative ideas in applied physics [1]. It is novel instrument for theoretical and computation research in class of problems named physical kinetics. It is a balance equation for distribution function – a density of some sort particles in their phase space [2], [3]. Compared with hydrodynamical problems the space dimension for field arguments is not equal 3, but 6. Of course, it makes difficulties in computation of solution.

To avoid large dimension in use the Boltzmann equation for electron gas in plasma physics they used, together with local approach [3], [4], to apply so named the Lorentz two term approximation (LTTA) for electron distribution function (EDF) [4]:

\[ f(v) = f_0(v) + f_1(v) \cdot v, \quad v = |v|. \]

This approach leads to hydrodynamical drift and diffusion equations for electron gas component in plasma. As electron is very light, in many situations EDF is approximately isotropic. Present-day the A.V. Phelps JILA bases (and other bases) [5] – [7] of electron cross-sections and transport properties are calculated in this approximation for EDF.

However there exists a class of problems, in which LTTA is not sufficient. In rare systems, such as low pressure glow discharge and hollow cathode, EDF can be significantly nonlocal and anisotropic. Simplest example is a problem about the wall absorbing electrons: what is EDF near this wall?

2. Statement of the Problem

Consider a problem:

\[ \xi = \cos \theta \] is a cosine of slope angle between direction of electron motion and \( x \) -axis; \( x = 0 \) is a wall. The equation includes an operator of low-angle scattering of electrons on gas molecules, the transport rate coefficient is equal to unit. To simplify situation the electric field assumed to be absent. The asymptotic (3) at large distance from the wall satisfies the kinetic equation (1), but does not satisfy the wall boundary condition (2), so the solution

\[ f(0, \xi) = 0, \quad \xi > 0; \]

\[ f(x, \xi) \rightarrow \frac{1}{2}(x - \xi + c), \quad x \rightarrow \infty. \]

It is a dimensionless kinetic equation for electrons having velocity \( v = 1 \) in 3D half-space \( x > 0 \) of ionized gas, molecules and ions of which having small velocity and large mass compared with electrons; \( \xi = \cos \theta \) a cosine of slope angle between direction of electron motion and \( x \) -axis; \( x = 0 \) is a wall. The equation includes an operator of low-angle scattering of electrons on gas molecules, the transport rate coefficient is equal to unit. To simplify situation the electric field assumed to be absent. The asymptotic (3) at large distance from the wall satisfies the kinetic equation (1), but does not satisfy the wall boundary condition (2), so the solution

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1 This is possible nearby the anode wall in glow discharge, when a probability of ion recombination in the anode is rather small, ions mostly are reflected, but some electrons and ions neutralize each other.
of the problem has additional summands, which are to be found. Also the constant $c$ in (3) is to be found. The problem has no parameters, so it is fundamental.

In some physical sense the problem is similar to so named the Milne problem [8]: to find a distribution function at the absorbing wall for particles, which are scattering in a law for elastic solid balls. In mathematics of the Milne problem a finite value of total scattering cross-section is significant. So the collision integral in kinetic equation can be presented as a sum of two terms: the input integral term – for particles, which get given velocity before scattering; and output term – for particles, which had given velocity before scattering and change it after scattering. If the differential cross-section does not depend on the angle of scattering, the Milne problem can be reduced to the Wiener and Hopf kind integral equation for a density of particles [9] with the Hopf kernel. Wiener and Hopf develop special method to solve this equation with use of analytical properties of the Fourier transformation of the equation and its solution. One can obtain analytic expression for solution of this problem and numerical values of its principal points (see Appendix at the end).

Application of the Milne problem is a propagation of light in muddy medium, and neutrons in solids and liquids. The electron scattering in plasma gives other type of collision term and needs other approach to solve problem, because total scattering cross-section for electrons is infinite.

3. The Legendre Polynomial Expansion

Let us find an approximation of solution in a form:

$$f(x, \xi) = \sum_{n=0}^{N} f_{2n}(x)P_{2n}(\xi) + \sum_{n=0}^{N} f_{2n+1}(x)P_{2n+1}(\xi).$$

Substitution and use the Legendre polynomial properties leads to the equation system:

$$\begin{align*}
2m+1 \frac{d f_{2m}}{dx} + 2(m+1) \frac{d f_{2m+1}}{dx} + (2m+1)(m+1) f_{2m+1} &= 0; \\
4m+1 \frac{df_{2m}}{dx} + 4(m+1)\frac{df_{2m+1}}{dx} + (m+1)\frac{df_{2m+1}}{dx} &= 0; \\
2m \frac{d f_{2m+1}}{dx} + 2m+1 \frac{df_{2m+1}}{dx} + m(2m+1) f_{2m} &= 0.
\end{align*}$$

$$m = 0,1,\ldots,N; \quad f_{2N+2} \equiv f_{-1} \equiv 0.$$

Boundary condition (2) in the wall gives

$$f_{2m}(0) = \sum_{n=0}^{N} B_{mn} f_{2n+1}(0), \quad m = 0,\ldots,N.$$  (6)
\[ f(x) = \frac{1}{2} x t_0 + \frac{1}{2} t_0' + T e^{-\lambda_N} p, \]
\[ e^{-\lambda_N} = \text{diag}(e^{-\lambda_0}, \ldots, e^{-\lambda_N}), \]
\[ p = (p_0, \ldots, p_N)^T, \quad T = (t_0, t_1^{(-)}, \ldots, t_N^{(-)}), \]
\[ \dim T = 2(N+1) \times (N+1). \]
\[ t_0 = (1, 0, \ldots, 0)^T, \quad M t_0 = 0; \]
\[ t_0' = (0, \ldots, 0, -1, 0, \ldots, 0)^T, \quad M t_0' = t_0; \]
\[ M t_n^{(-)} = -\lambda_n t_n^{(-)}, \quad n = 1, \ldots, N. \]

With use of boundary condition (6) – (7), the vector \( p \) can be found as a solution of algebraic system
\[ (B'T' - T)p = \frac{1}{2} b_0. \] (11)

Here \( b_0 \) is first column in matrix \( B \) in (7), \( B' \) is matrix \( B \) without first column,
\[ f_i(0) = T_i p, \quad \dim T = (N+1) \times (N+1); \]
\[ f_i'(0) = T'_i p, \quad \dim T' = N \times (N+1). \] (12)

In (12) “+” and “-” subscripts denote upper and lower half of a matrix, sign “´” denotes an exclusion of first row of a matrix. After calculation of the vector-column \( p \) the solution can be found by substitution \( p \) into (10), and \( f(x) \) into (4).

4. Results and discussion

If one uses \( N = 50 \) (102 Legendre polynomials), one can obtain a result shown on Fig. 1. The EDF is rather good quality, oscillating deviations from zero at positive values of \( \xi \) (directions inward plasma volume) are small enough to believe that the approximation of solution is good. Fig. 2 illustrates a density of electrons nearby the wall. In nearest points the density deflects from linear dependence upon \( x \) to more low value.

One can ask a question: why the Legendre polynomials are used here, if one can use the Fourier method of variable separation to find a basic solutions for operator in (1)? – Formally it could be right (and standard) way. But really the eigenfunctions in the Fourier approach is more difficult to calculate (see Fig. 3) because of their complicated behavior especially for high modes. To calculate these modes in amount bigger then 10 with good accuracy – is not easy problem. But the Legendre polynomials are well defined: their coefficients are rational numbers, and formulas are well known. On Fig. 4 the maximal deviation of EDF on the wall from zero at positive \( \xi \) is presented. One can see: the accuracy rises with a number of polynomials, though not very fast. Also the calculation time rises because of size of matrices.
more difficult. These calculations enable to hope that a sequence of approximations converge to true solution.

5. Conclusion

The multi-term approximation, based on finite Legendre polynomial expansion by cosine of slope angle to axis of system symmetry, enables to solve an anisotropic problem with accuracy much greater then traditional the Lorentz two term approximation for electron distribution function in physical kinetics of plasma. It worse to mention, that an infinite Legendre polynomial expansion of EDF is not creative, because the infinite ODE system of equations, analogues to (5), cannot be resolved with regard to the derivatives and leads to deadlock.

APPENDIX

1. Uniqueness of a solution.

Theorem. If a solution of problem (1) – (3) exists, it is unique.

The proof. If there exist two solutions of problem (1) – (3): \( f_1(x, \xi), f_2(x, \xi) \), then function

\[ h(x, \xi) = f_1(x, \xi) - f_2(x, \xi) \]

is a solution of the problem:

\[ \xi \frac{\partial h}{\partial x} = \frac{1}{2} \left( \frac{\partial h}{\partial \xi} \right) (1 - \xi^2), \quad 0 < x < \infty, \quad -1 < \xi < 1; \]

\[ h(0, \xi) = 0, \quad \xi > 0; \]

\[ h(x, \xi) \rightarrow \Delta = \frac{1}{2} (c_2 - c_1), \quad x \rightarrow \infty. \]

Let us multiply the equation (14) by \( h(x, \xi) \) and integrate over the variable \( \xi \) within \(-1, +1\). After some transformations we get:

\[ \frac{\partial}{\partial x} \int_{-1}^{1} d\xi \left( \xi^2 \frac{h^2}{2} \right) = \frac{1}{2} \int_{-1}^{1} d\xi \frac{\partial}{\partial \xi} \left( 1 - \xi^2 \right) \left( \frac{\partial h}{\partial \xi} \right)^2, \quad 0 < x < \infty; \]

\[ \frac{\partial}{\partial x} \int_{-1}^{1} d\xi \left( \xi h^2 \right) = \]

\[ = \int_{-1}^{1} d\xi \frac{\partial}{\partial \xi} \left( 1 - \xi^2 \right) h \frac{\partial h}{\partial \xi} - \int_{-1}^{1} d\xi \left( 1 - \xi^2 \right) \left( \frac{\partial h}{\partial \xi} \right)^2; \]

\[ \frac{dH}{dx} = -\int_{-1}^{1} d\xi \left( 1 - \xi^2 \right) \left( \frac{\partial h}{\partial \xi} \right)^2 \leq 0, \quad 0 < x < \infty; \]

\[ H(x) = \int_{-1}^{1} d\xi \left( \xi h^2(x, \xi) \right). \]

By virtue of (15) and (16) we have:
\[ H(0) = \int_{-1}^{+1} d\xi (\xi^2(0, \xi)) = \frac{1}{2} \int_{-1}^{+1} d\xi (\xi^2(0, \xi)) \leq 0; \quad (18) \]

\[ \lim_{x \to \infty} H(x) = \lim_{x \to \infty} \int_{-1}^{1} d\xi (\xi^2(x, \xi)) = \int_{-1}^{1} d\xi (\xi^2(0, \xi)) = 0. \quad (19) \]

Thus, we have found, that the continuously differentiable function
\[ H(x) = \int_{-1}^{1} d\xi (\xi^2(x, \xi)), \quad 0 \leq x < \infty \quad (20) \]
has non-positive value at \( x = 0 \), by virtue of (18). On the other hand, by virtue of (17), it does not increase with a growth of \( x \), and tends to the limit equal to zero when \( x \) approaches infinity. All of this is possible only in case when
\[ H(x) = 0, \quad 0 \leq x < \infty. \quad (21) \]

Then from (15), (18) and (21) it follows
\[ h(0, \xi, 0) = 0, \quad -1 < \xi < +1; \quad (22) \]
Also from (17) and (21) we obtain
\[ \frac{\partial h}{\partial \xi}(x, \xi) = 0, \quad -1 < \xi < +1, \quad 0 < x < \infty. \quad (23) \]

By substituting (23) into equation (14) we have
\[ \frac{\partial h}{\partial \xi}(x, \xi) = 0, \quad -1 < \xi < +1, \quad \xi \neq 0, \quad 0 < x < \infty. \quad (24) \]

From (22), (23) and (24), also taking into account a continuity of differentiable function \( h \) in the boundary \( x = 0 \) of its domain of definition, also in the half-axis \( \xi = 0, \quad 0 \leq x < \infty \), it follows:
\[ h(x, \xi) = \text{const} = 0, \quad -1 \leq \xi \leq +1, \quad 0 \leq x < \infty. \quad (25) \]

Thus, a difference in any two solutions of the problem (1) – (3), if these solutions exist, is equal to zero. Therefore, a solution is unique. The theorem is proved.


For a distribution function
\[ f = f(x, \cos \vartheta), \quad (26) \]
which is a density \( M \) in a six-dimensional phase space of spatial coordinates and velocities
\[ dM = f(x, \cos \vartheta) \delta(v' - v) dx dy dz dv_x dv_y dv_z, \quad (27) \]
let us write a stationary kinetic (or the Boltzmann) equation
\[ \psi' = \frac{2\pi \psi}{-3J} f(x, \cos \vartheta) \quad (32) \]

In these new values (omitting sign "'"") we rewrite the problem in the form:
\[ \xi \frac{\partial f}{\partial \xi} + f - \frac{1}{2} \int_{-1}^{1} d\xi' f(x, \xi') = 0, \]  
\( x > 0, \; -1 \leq \xi \leq 1; \)  
\( f(0, \xi) = 0, \; 0 < \xi \leq 1; \)  
\( f(x, \xi) \geq 0, \; x \geq 0, \; -1 \leq \xi \leq 1; \)  
\[ \int_{-1}^{1} d\xi \xi f(0, \xi) = -\frac{1}{3}. \]  
(33)  
(34)  
(35)  
(36)

It is the Milne problem in its canonical form.

Solution.

Introducing dimensionless particle density
\[ n(x) = \int_{-1}^{1} d\xi f(x, \xi), \]  
(37)

one considers (33) as an ordinary differential equation on variable \( x \):
\[ \xi \frac{df}{dx} + f = \frac{1}{2} n(x). \]  
(38)

One integrates it with use of a variation of constant method [10] and transforms into an integral equation. Most simple form is
\[ f(x, \xi) = \frac{1}{2} \int_{0}^{\infty} dy e^{-\tau} n(x - y\xi), \; \xi < 0; \]  
(39)  
\[ f(x, \xi) = \frac{1}{2} \int_{0}^{\infty} dy e^{-\tau} n(x - y\xi), \; \xi > 0; \]  
(40)  
\[ f(x, 0) = \frac{1}{2} n(x). \]  
(41)

Here \( n \) is meant as taken from (37). The form (39) satisfies automatically boundary condition (34) in the wall at \( x = 0 \).

It is possible, however, instead of integral equation for two variable function \( f(x, \xi) \), to build an integral equation for one variable function \( n(x) \). To do this, let us integrate (39) and (40) by variable \( \xi \) and substitute a sum of results into left-hand side of (37). After transformations of integration variables we get an equation:
\[ n(x) = \frac{1}{2} \int_{0}^{\infty} dx' n(x') \text{Ei}(-|x - x'|). \]  
(42)

Here a special function, the integral exponential function [11], is used:
\[ \text{Ei}(z) = \int_{-\infty}^{z} \frac{e^t}{t} dt, \; z < 0. \]  
(43)

Condition of distribution function non-negativity (35) gives a condition of non-negativity for \( n(x) \):
\[ n(x) \geq 0. \]  
(44)

Condition for a flux density (36) gives a condition for normalization of \( n(x) \):
\[ \int_{0}^{\infty} dx n(x) e^{-x} + x \text{Ei}(-x) = \frac{2}{3}. \]  
(45)

The equation (42) is named the Milne equation [12] and has mathematical type of the Wiener-Hopf kind equation in the literature [13].

Wiener and Hopf developed special method for solving of linear integral equations, having a kernel, which depends on difference of its arguments, and when limits of integration are zero and infinity [14]. For the Milne problem it is possible to obtain an analytical expression for solution of the equation (42) under normalization (45):
\[ n(x) = \frac{1}{2\pi} \int_{\mu < 1} dk \frac{k^{-1}}{k^2 - \beta} \times \exp \left\{ \frac{i k}{2\pi} \int_{0}^{\infty} d\eta \frac{1}{\eta} \ln \left( 1 + n^2 \eta \left( \frac{1}{\eta} - \frac{\text{arctg} \eta}{\eta} \right) \right) - i k x \right\}, \]  
(46)

Here complex normalization factor is chosen in such way, that a solution would be real and satisfy condition (45). Constants \( \beta, \mu \), which define positions of paths of integration in the complex plane, can be varied in limits defined – in such manner, that the paths would not cross singular points of integrands. According to the Cauchy theorem [14], such variation does not change a result.

However the formula (46) contains one exiting thing: if you merely write it in some mathematical package, the “Wolfram Mathematica 9.0” for example, and plot a picture of the solution, you would have something like Fig. 7.

To make correct calculations of two integrations in (46) – is a problem, which needs additional inventions and efforts. It seems, that more easy way is to use a finite element method (FEM) [15]. It is possible if you know asymptotic behavior of solution at \( x \to \infty \). In this way one can obtain a picture like Fig. 8.
The accuracy of the Galerkin finite element method is much better than attempts to use analytic formula (46) for calculations of \( n(x) \), – see Fig. 9, 10. One can see that at number of elements equal to 1000 the accuracy of the FEM is better than 0.001. This can satisfy most of wishes for physicists and experimentalists.

But the analytic (!) formula (46) gives (with good luck) something like the Fig. 11.

Nevertheless the Wiener-Hopf method gives good way to calculate the distribution function of particles in the wall: at \( x = 0 \). If we take the Fourier transformation term from (46)

\[
U_s(k) = \frac{1}{\sqrt{2\pi}} \frac{ik - 1}{k^2} \times
\exp \left( -k \int -\alpha \beta \frac{d\eta}{\eta(\eta - k)} \ln \left( \frac{1 + \eta^2(1 - \text{arctg}\eta)}{\eta} \right) \right),
\]

\( 0 < \beta < 1 \),

we can calculate \( f(0, \xi) \) by formula
\[ f(0, \xi) = \sqrt{\frac{\pi}{2 - \xi}} U_{0}(\frac{i}{\xi}), \quad \xi < 0; \quad (48) \]
\[ f(0, \xi) = 0, \quad \xi > 0. \quad (49) \]

The picture of this dependence is presented on Fig. 12. In comparison with Fig. 1 (red curve) one can see, that the Milne problem with solid balls (Fig. 12) gives a discontinuous dependence of \( f \) on cosine of slope angle – with a jump at a direction of particles parallel to the wall, – as far as slow-angle scattering gives a continuous dependence (Fig. 1).

![Image](image.png)

**Fig. 12. Calculation \( f(0, \xi) \) with the Wiener-Hopf method.**

By integration (48) over cosine of slope angle one can obtain a value of density \( n \) in the wall:

\[ n(0) = \int_{-1}^{0} d\xi \ f(0, \xi) \approx 0.577350272... \quad (50) \]

Formula (46) helps also to find an asymptotic behavior of density \( n \) at large values of \( x \). If we extract a singular part of (47) near the point \( k = 0 \) we can obtain

\[ U_{+}^{s}(k) = \frac{1}{\sqrt{2\pi}} \left( \frac{-1}{k^{2}} + i \frac{C}{k} \right) \quad (51) \]

The reverse Fourier transformation of (51) gives the asymptote for \( n(x) \) at \( x \to \infty \)

\[ n^{(s)}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk U_{+}^{s}(k) e^{-ikx} = x + C. \quad (52) \]

Here \( C \) is the Hopf constant [16]

\[ C = 1 - \frac{1}{2\pi} \int_{-\infty}^{\infty} d\eta \frac{q(\eta - i\beta)}{\eta - i\beta} \approx \]
\[ \approx 0.7104460895987215... \quad (53) \]

\[ q(k) = \ln \left( \frac{1 + k^{2}}{k^{2}} \left( 1 - \frac{\arctg k}{k} \right) \right) \quad (54) \]

The comparison of two utmost variants of particle scattering nearby absorbing wall: solid balls (with finite total cross-section) and far-interacted low-angle scattered (with infinite total cross-section), – shows what is common and what is different. The results on particle density \( n \) are close each other, but the angle distribution behavior of \( f \) at the wall is different: discontinuous and continuous. Probably, all intermediate variants of scattering are located within these limits.

**References**


