Nonlinear theory of ion stopping in classical plasmas: Application to the Barkas effect

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A nonlinear theory of ion stopping in classical ideal plasmas is formulated on the basis of formalism of higher-order dielectric functions accounting for nonlinear relationship between polarization and electric fields generated in plasma by the projectile ion. Corrections to the linear theory corresponding to the Barkas effect are evaluated explicitly. The result differs (what concerns the numerical coefficient) from that following from the harmonic oscillator model.

1. Introduction

The well-known dielectric theory of energy losses of an ion in plasmas is based upon the assumption of linear relationship between polarization $P$ and electric field $E$ generated by the ion. The assumption of linearity can, however, break down if the charge $e_p$ of the projectile ion is high and, therefore, fields generated around it are strong. In this case, it is necessary to take into account higher-order terms in the expansion of $P$ in the field strength $E$. The coefficients in this expansion represent higher-order susceptibilities of a plasma. The knowledge of these susceptibilities, which are widely used in nonlinear electrodynamics (see, e.g., Sitenko 1982) allows one to formulate the problem of nonlinear stopping of highly charged ions in different plasmas in the most adequate way. This approach is equivalent, of course, to the Green function technique used in Sung & Ritchie (1983) for calculation of stopping power of quantum electron gas for fast ions. However, the dielectric formalism developed below appears to be much more simple.

We will restrict ourselves here to the classical ideal plasmas described by the Vlasov equation defining an electron distribution function $f_0 + f$, $f_0$ being undisturbed (Maxwellian) distribution function.

Introducing Fourier components $f_{k\omega}$, $E_{k\omega}$ we can write the Vlasov equation as follows:

$$-i(\omega - kv)f_{k\omega} + \frac{e}{m} E_{k\omega} \frac{\partial f_0}{\partial v} + \frac{e}{m} \int \frac{d\omega'}{(2\pi)^3} E_{k'\omega'} \frac{\partial f_{k-k':\omega'-\omega}}{\partial v} = 0 \quad (1)$$

where $e$, $m$, $v$ are the charge, mass, and velocity of the plasma electrons. The Fourier components $f_{k\omega}$ can be represented by expansion in ascending powers of $E_{k\omega}$, $f_{k\omega} = \sum_{n=1}^{\infty} f_{k\omega}^{(n)}$, where

$$f_{k\omega}^{(1)} = -i \frac{e}{m} \frac{1}{\omega - kv} E_{k\omega} \frac{\partial f_0}{\partial v}, \quad f_{k\omega}^{(n)} = \frac{e}{m} \frac{-i}{\omega - kv} \int \frac{d\omega'}{(2\pi)^3} E_{k'\omega'} \frac{\partial f_{k-k':\omega'-\omega}}{\partial v}. \quad (2)$$

Inserting this expansion in the Fourier-transformed Poisson equation

$$i k E_{k\omega} = 4\pi \left( e \int f_{k\omega} dv + \rho_{k\omega}^{(0)} \right), \quad (3)$$
where $\rho_{k\omega}^0 = 2\pi e_p \delta(\omega - k\nu_p)$ is the charge density corresponding to the projectile ion having velocity $\nu_p$, and introducing the polarisation vector $P_{k\omega}$ by the relation $i k P_{k\omega} = 4\pi e \int f_{k\omega} d\nu$ we get the basic nonlinear equation for the field $E_{k\omega}$ in the plasma

$$i k (E_{k\omega} + P_{k\omega}) = i k \left[ \varepsilon(k, \omega) E_{k\omega} + \int \frac{d\omega_1 \, dk_1}{(2\pi)^4} \chi^{(2)}(k, \omega_1, \omega_2) + \cdots \right] = 4\pi \rho_{k\omega}^0, \quad (4)$$

where $\varepsilon = 1 + \chi^{(1)}$ and $\chi^{(n)}$, $n = 2, 3, \ldots$ are the plasma susceptibilities of different order. For $n = 1, 2$, they are given by the formulas

$$\chi^{(1)} = \frac{\omega_p^2}{k^2} \int \frac{k \, df_0}{\omega - k\nu} = \frac{k_d^2}{k^2} \left[ 1 + s Z(s) \right], \quad k_d = \frac{\omega_p}{\nu}, \quad f_0 = N f_0, \quad (5)$$

where $\omega_p = (4\pi N e^2 / m)^{1/2}$ is the plasma frequency, $N$ being the plasma electron density, $Z(s)$ is the plasma dispersion function, $s = \omega / \sqrt{2 \mu k}$, $\nu = (T/m)^{1/2}$;

$$\chi^{(2)}(\omega_1, k_1, \omega_2, k_2) = -\frac{i}{2} \frac{e\omega_p^2}{(k) m} \int \frac{d\nu}{\omega - k\nu} \left( k_1 \frac{\partial}{\partial \nu} k_2 \frac{\partial}{\partial \nu} \right) A(k) f_0, \quad (6)$$

where

$$\omega = \omega_1 + \omega_2, \quad k = k_1 + k_2, \quad (k) = k_1 k_2 k.$$

Neglecting in the first approximation nonlinear terms in (4), we get the first-order Fourier component of the field in the plasma:

$$E_{k\omega}^{(1)} = -\frac{4\pi i \rho_{k\omega}^0}{k \varepsilon(\omega, k)}. \quad (7)$$

Second-order fields are defined now, according to (4), by the formula

$$E^{(2)} = -\frac{\int \chi^{(2)}(k_1, \omega_1) E_{k_2, \omega_2}^{(1)} \frac{d\omega_1 \, dk_1}{(2\pi)^4}}{\varepsilon(\omega, k)}, \quad (8)$$

where $E_{k_1, \omega_1}^{(1)}$ are first-order fields given by (7). We can now formulate a general expression for the stopping power $W$, i.e., for the energy loss of an ion per a unit length of its straight path, as follows:

$$W = \frac{e_p}{v_p} (E_{k\omega, j}) = \frac{e_p}{v_p} \left[ \sum_{n=1}^{\infty} E^{(n)} \cdot v_p \right]$$

$$= \frac{e_p^2 i}{2 \pi^2 v_p} \int \frac{\omega \, dk}{k^2} \left[ \frac{1}{\varepsilon(\omega, k)} - 1 \right] + \frac{e_p^3}{(2\pi^2)^2 v_p} \int \frac{\omega \chi^{(2)}(\omega_1, \omega_2, k_1, k_2) \, dk_1 \, dk_2}{(k) (\varepsilon)} + \cdots \quad (9)$$

where

$$(\varepsilon) = \varepsilon_1 \varepsilon_2 \varepsilon, \quad \varepsilon = \varepsilon(\omega, k), \quad \varepsilon_1 = \varepsilon(\omega_1, k_1), \quad \varepsilon_2 = \varepsilon(\omega_2, k_2), \quad \omega_{1,2} = k_{1,2} \nu_p.$$

[We substracted in (9) self-field of the ion.]
The second term in this expansion represents the Barkas correction $W_B$. Higher-order terms can be easily formulated with the help of expressions for $\chi^{(n)}$, $E^{(n)}$ given in Sitenko (1982). In the following, we will derive an explicit expression for $W_B$ restricting ourselves with limiting case $v_p \gg u$.

2. Barkas correction for fast ions, $v_p \gg u$

In the case $v_p \gg u$, we can consider in the expression (6) for $\chi^{(2)}$ the terms $k_{1,2} v$ as small compared to respective $\omega_{1,2}$. We get in this way, performing an expansion over $k_{1,2} v$ in (6), the following formula for $\chi^{(2)}$ (see Sitenko 1982, p. 25):

$$\chi^{(2)} = -\frac{i}{2} \frac{e \omega_p^2}{m \omega_1 \omega_2 \omega(k)} \left[ \frac{k_1^2(k_2)}{\omega_1} + \frac{k_2^2(k_1)}{\omega_2} + \frac{k_1^2(k_2)}{\omega} \right], \quad (k) = k_1 k_2 k. \quad (10)$$

Corrections to (10) (Sitenko 1982, p. 25) due to the electron thermal motion are of the order of $u^2/v_p^2$.

Inserting this expression into formula (9) for $W_B$, we get

$$W_B = \frac{e^2 \omega_p^2 \nu}{2(2\pi^2)^2 mv_p}, \quad y = y_1 + y_2 + y_3, \quad y_1 = -i \int \frac{(kk_2)}{\omega_1^2 \omega_2 k^2 k_2^2(e)} \, dk_1 \, dk_2, \quad (11)$$

$$y_2 = -i \int \frac{(kk_1)}{\omega_2^2 \omega_1(e)k_1^2 k_2^2} \, dk_1 \, dk_2, \quad y_3 = -i \int \frac{(kk_1)}{\omega_1 \omega_2(e)k_1^2 k_2^2} \, dk_1 \, dk_2.$$

According to the assumptions $k_{1,2} v \ll \omega_{1,2}$ used above, we can neglect space dispersion and write the dielectric functions $\epsilon_{1,2}, \epsilon$ in the form $\epsilon_{1,2} = \epsilon_{1,2}(\omega_{1,2}), \epsilon = \epsilon(\omega)$. Introducing instead of $k_1$, $k_2$ new variables $q_1, q_2, \phi_{1,2}, \omega_{1,2}/v_p$ connected with $k_1, k_2$ by the relations $k_{1,2}^2 = q_{1,2}^2 + (\omega_1^2/\omega_p^2)$ (thereby we have also $dk_1, dk_2 = dq_1, dq_2, d\phi_{1,2}, d\omega_{1,2}/v_p$) and performing integrations over $\phi_{1,2}$, thus eliminating in $k_1 k_2 = q_1 q_2 \cos(\phi_1 - \phi_2) + \omega_1 \omega_2/v_p^2$ (as well as in $kk_1$) the terms containing $\phi_{1,2}$, we get

$$y_3 = \frac{1}{v_p^2} \int \frac{dk_1 \, dk_2}{\omega k_1^2 k_2^2} \left( \frac{2\eta_1 \epsilon' \epsilon_2'}{\epsilon \epsilon_2} + \frac{\eta \epsilon_2}{\epsilon \epsilon_2'} \right), \quad (12)$$

$$y_1 = y_2 = \frac{1}{v_p^2} \int \omega dk \, dk_1 \left( \frac{\eta_1 \epsilon' \epsilon_2'}{\epsilon \epsilon_2} + \frac{\eta \epsilon_2}{\epsilon \epsilon_2'} \right). \quad (13)$$

Here, $\phi_{1,2}$ are polar angles specifying the vectors $q_{1,2}$ in the plane perpendicular to $v_p$, $\epsilon_{1,2}', \epsilon'$ are real parts of $\epsilon_{1,2}, \epsilon$ and $\eta_{1,2}, \eta$ are imaginary parts of $1/\epsilon_{1,2}, 1/\epsilon$. [We used in (13) the transformation $dk_1 \, dk_2 = dk \, dk_1$, and the fact that the integrals in (12) involving $\eta_1 \epsilon' \epsilon_2'$ and $\eta_2 \epsilon' \epsilon_1'$ are identical.] Within the cold plasma approximation, the functions $\epsilon', \eta$ are equal to: $\epsilon' = 1 - (\omega_2^2/\omega^2)$, $\eta = -(\pi \omega_p/2) [\delta(\omega - \omega_p) - \delta(\omega - \omega_p)]$. The integrals over $\omega_1$, $\omega_2$, $\omega$ must be understood in a sense of their principal values. [It is necessary to stress that this way of simplification of the integrals in (11) is only possible in the cold plasma approximation—only in this case do the dielectric functions $\epsilon_{1,2}, \epsilon$ not depend upon respectively $k_{1,2}$, $k$ and hence, on the azimuthal angles $\phi_1, \phi_2$. Note also that in this approximation the terms in (12), (13) involving the product $\eta_1, \eta_2, \eta$ disappear because they prove to be proportional, after an integration over $\omega_1, \omega_2$, to $\delta(\omega_1 + \omega_2 - \omega_p)$, where $\omega_{1,2} = \pm \omega_p$ and, hence, they are equal to zero for any combination of the signs $\pm$.]

Performing in (12) and (13) integrations over $q_{1,2}$ in an interval $0 < q_{1,2} < q_m$, $q_m$ being a maximal value of $q_{1,2}$, we arrive at the formulas: $y_3 = y_3^{(1)} + y_3^{(2)}, y_1 = y_1^{(1)} + y_1^{(2)} + y_1^{(3)}.$
Yu. S. Sayasov

\[ y_3^{(1)} = \frac{2}{u_p^2} \int \frac{\eta_1 \, dk_1 \, dk_2}{\omega k_1^2 k_2^2 e^2} = -\frac{8\pi^3 \omega_p \ln \Lambda_0}{u_p^4} \int_{-\infty}^{\infty} \frac{\ln \Lambda(\omega) \, d\omega}{\varepsilon(\omega)\varepsilon(\omega + \omega_p)(\omega + \omega_p)} \]

\[ y_3^{(2)} = \frac{1}{u_p^2} \int \frac{\eta_1 \, dk_1 \, dk_2}{\omega k_1^2 k_2^2 e^2} = -\frac{4\pi^3 \omega_p \ln \Lambda_0}{u_p^4} \int_{-\infty}^{\infty} \frac{\ln \Lambda(\omega) \ln \Lambda(\omega + \omega_p) \, d\omega}{\varepsilon(\omega)\varepsilon(\omega + \omega_p)} \]

\[ y_1^{(1)} = \frac{1}{u_p^2} \int \frac{\eta_1 \, dk \, dk_1}{\omega^2 e^2 k^2 k_1^2} = \frac{4\pi^3 \omega_p \ln \Lambda_0}{u_p^4} \int_{-\infty}^{\infty} \frac{\ln \Lambda(\omega) \, d\omega}{\varepsilon(\omega)\varepsilon(\omega + \omega_p)(\omega + \omega_p)^2} \]

\[ y_1^{(2)} = \frac{1}{u_p^2} \int \frac{\eta \, dk \, dk_1}{\omega^2 e^2 k^2 k_1^2} = -\frac{4\pi^3 \omega_p^2 \ln \Lambda_0}{u_p^4} \int_{-\infty}^{\infty} \frac{\ln \Lambda(\omega) \, d\omega}{\varepsilon(\omega)\varepsilon(\omega + \omega_p)(\omega + \omega_p)^2} \]

\[ y_1^{(3)} = \frac{1}{u_p^2} \int \frac{\eta_2 \, dk_1 \, dk_1}{\omega^2 e^2 k_1^2 k^2} = \frac{4\pi^3}{u_p^4 \omega_p} \int_{-\infty}^{\infty} \frac{(\omega + \omega_p) \ln \Lambda(\omega) \ln \Lambda(\omega + \omega_p) \, d\omega}{\varepsilon(\omega)\varepsilon(\omega + \omega_p)} \]

where \( \Lambda_0 = [(q_m v_p^2/\omega_p^2) + 1]^{1/2} = q_m v_p/\omega_p, \Lambda(\omega) = [(q_m v_p^2/\omega^2) + 1]^{1/2}, \varepsilon(\omega) = 1 - (\omega^2/\omega_p^2). \) Combining these integrals, we can rewrite the expression \( y \) entering into (11) as follows:

\[ y = y_1 + y_2, y_1 = y_3^{(1)} + 2(y_1^{(1)} + y_1^{(2)}), y_2 = y_3^{(2)} + 2y_1^{(3)} \]

\[ j_1 = \frac{16\pi^2 \ln \Lambda_0}{u_p^2} \int_{-\infty}^{\infty} \frac{\ln \Lambda(\omega) \, d\omega}{\varepsilon(\omega)\varepsilon(\omega + \omega_p)(\omega + \omega_p)^2} \]

\[ j_2 = \frac{4\pi^3}{u_p^2 \omega_p} \int_{-\infty}^{\infty} \frac{(2\omega + \omega_p) \ln \Lambda(\omega) \ln \Lambda(\omega + \omega_p) \, d\omega}{\varepsilon(\omega)\varepsilon(\omega + \omega_p)} = \frac{4\pi^3}{u_p^2 \omega_p} I. \]

The integral \( j_2 \) appears to be equal to zero, as shown following elementary transformations. Introducing the ratio \( \ln \Lambda(\omega)/\varepsilon(\omega) = \Psi(\omega) \), using the property \( \Psi(-\omega) = \Psi(\omega) \) and substitutions \( \omega + \omega_p = \nu, \nu = -\alpha \), we can rewrite the integral

\[ = \int_{-\infty}^{\infty} \omega \Psi(\omega) \Psi(\omega + \omega_p) \, d\omega \]

in \( j_2 \) as

\[ = \int_{-\infty}^{\infty} (\nu - \omega_p) \Psi(\nu) \Psi(\nu - \omega_p) \, d\nu = \int_{-\infty}^{-\infty} (\alpha + \omega_p) \Psi(\alpha) \Psi(\alpha + \omega_p) \, d\alpha \]

\[ = -\int_{-\infty}^{\infty} (\omega + \omega_p) \Psi(\omega) \Psi(\omega + \omega_p) \, d\omega. \]

This means that

\[ I = \int_{-\infty}^{\infty} (2\omega + \omega_p) \Psi(\omega) \Psi(\omega + \omega_p) \, d\omega = 0, \]

i.e., \( j_2 = 0 \) or \( y = j_1 \).

We can, hence, express the stopping power defined by (11) as follows:

\[ W_B = \frac{2e_p^3 \omega_p^3 \ln \Lambda_0}{\pi m v_p^5} \int_{-\infty}^{\infty} \frac{\ln \Lambda(\omega) \, d\omega}{\varepsilon(\omega)\varepsilon(\omega + \omega_p)(\omega + \omega_p)^2} = \frac{2j_e^3 e_p^3 \omega_p^3 \ln \Lambda_0}{\pi m v_p^5}. \]

Note that the remarkably simple formula (14) representing \( W_B \) by a single integral over \( \omega \) corresponds to the hydrodynamical approximation (see Sitenko 1982, p. 25).
The constant $j$ is given by

$$j = \int_{-\infty}^{\infty} \frac{\ln x^2 \, dx}{\varepsilon(x)\varepsilon(x + 1)(x + 1)^2} = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\ln x^2 \cdot x \, dx}{(x^2 - 1)(x + 2)}$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} \ln x^2 \left[ \frac{1}{3(x - 1)} - \frac{4}{3(x + 2)} + \frac{1}{x + 1} \right] \, dx.$$  

We assumed here that $\ln A = \frac{\ln(A_0/x^2)}{2}$ and used the fact that the principal value of the integral

$$\int_{-\infty}^{\infty} \frac{dx}{\varepsilon(x)\varepsilon(x + 1)(x + 1)^2}$$

is equal to zero.] Transformations

$$\int_{-\infty}^{\infty} \frac{\ln x^2}{x + 1} \, dx = \int_{-\infty}^{\infty} \frac{\ln x^2 \, dx}{x - 1} = \int_{0}^{\infty} \ln x^2 \left( \frac{1}{x - 1} - \frac{1}{x + 1} \right) \, dx = 4 \int_{0}^{\infty} \frac{\ln x \, dx}{x^2 - 1} = \pi^2,$$

$$\int_{-\infty}^{\infty} \frac{\ln x^2}{x + 2} \, dx = \int_{-\infty}^{\infty} \frac{4\xi^2 \, d\xi}{\xi + 1} = \int_{-\infty}^{\infty} \frac{\ln \xi^2}{\xi + 1} \, d\xi = -\pi^2$$

lead now to the value $j = \pi^2/3$ and, hence,

$$W_B = \frac{2\pi}{3} \frac{e_p^3 \omega_p^2 \ln \Lambda_0}{m v_p^3}. \quad (15)$$

We can finally rewrite the expression for stopping power in the traditional form as follows:

$$W = -\frac{e_p^2 \omega_p^2}{v_p^2} \ln \Lambda + \frac{2\pi}{3} \frac{e_p^3 \omega_p^2 \ln \Lambda}{m v_p^3} = -\frac{e_p^2 \omega_p^2}{v_p^2} \left( \ln \Lambda + \frac{2\pi}{3} \frac{e_p \left| e \right| \omega_p}{m v_p^3} \ln \Lambda_0 \right), \quad (16)$$

where $\Lambda = 2m u_p^2/\hbar \omega_p$ (see e.g. Landau & Lifshits 1960).

Choosing the cutoff parameter $q_m$ as $q_m = m u_p/h$ (the value $q_m$ represents, evidently, a critical wave number above which quantum effects become important), we get $\Lambda_0 \equiv m v_p u_p/h \omega_p$, i.e., the value of $W_B$ that represents the contribution from distant projectile-plasma interactions. To take into account the contribution from close interactions of the projectile with the plasma electrons, one can choose, instead, the cutoff parameter as $q_m \equiv C m v_p/h$ (Lindhard 1976), thus arriving at the logarithmic factor $\ln(C m v_p^2/h \omega_p)$. (Numerical coefficient $C$ remains, however, poorly defined here.) It is necessary to stress that the numerical coefficient $2\pi/3 = 2.09$ in (16) differs from that $(3\pi/2 = 4.71)$ following from the elementary considerations in Lindhard (1976) and from the harmonic oscillator model of the Barkas effect (Ashley et al. 1972).

Further development of the theory of nonlinear corrections to the stopping power in the framework of the dielectric formalism sketched above would allow one to formulate, in particular, fully convergent theory incorporating the close interaction effects, i.e., by the method similar to that used by Maynard & Deutsch (1982) in linear electrodynamics. For this aim, it is necessary to develop quantum mechanical generalisation of the higher-order dielectric functions, which remains valid for high-wave numbers $k \approx q_m = m u_p/h$.

3. Conclusions

We developed a natural generalisation of the dielectric theory of energy losses of an ion in classical plasmas based upon using higher-order dielectric functions, allowing one to de-
scribe the nonlinear effects of different orders in a systematic way. The formula for the Barkas correction derived in this way differs (what concerns the numerical coefficient) from that following from the model of harmonic oscillator.

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