Dynamical conductivity of the Lorentz-Vlasov plasma

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Abstract. In the Lorentz-Vlasov model of a plasma the ions are assumed to be fixed in space with disordered distribution, and the Coulomb interaction between electrons is approximated by the Vlasov field, calculated self-consistently from the electron position-momentum distribution function. If correlations between ions are neglected, then the dynamical conductivity of the plasma may be evaluated from the dynamics of the electron gas in interaction with a single ion, the remaining ions being approximated by a uniform background. In dielectric or energy-loss theory the dynamical friction coefficient is expressed in terms of the dielectric function of the uniform electron gas. A more detailed theory must take full account of the scattering of electrons by the selected ion. It is shown for an electron gas at zero temperature and metallic density, and for a simple ion pseudopotential, that the frequency-dependence of the friction coefficient differs appreciably from that predicted by energy-loss theory.

1. Introduction
The aim of the work[1] presented here is to provide an accurate calculation of the dynamical conductivity $\sigma(\omega)$ of a plasma in linear response to an oscillating applied electric field, in classical approximation, and for strong coupling, with results valid over the full frequency range $0 < \omega < \infty$. The conductivity of a plasma is dominated by the motion of electrons colliding with the ions, which in good approximation may be assumed to remain static. Equivalently, we have therefore aimed to calculate the frequency-dependent electron-ion collision frequency $\nu_{ei}(\omega)$ or friction coefficient $\zeta(\omega) = m\nu_{ei}(\omega)$, where $m$ is the electron mass. The conductivity is expressed in these quantities as

$$\sigma(\omega) = \frac{n_0e^2/m}{-i\omega + \nu_{ei}(\omega)} = \frac{n_0e^2}{-i\omega + \zeta(\omega)},$$

where $n_0$ is the electron density, and $-e$ the electron charge.

In the Lorentz-Vlasov model the $N_i$ identical ions are fixed in space in disordered configuration of centers ($R_1, ..., R_{N_i}$), distributed according to a probability distribution $W(R_1, ..., R_{N_i})$, that is assumed known. The electrons are described by the Vlasov-equation for the one-electron distribution function $f(r, p, t)$, i.e. the structure of the electron system is neglected. In the following the electron-ion structure is taken into account for low density of ions. In principle the equilibrium ion-ion structure can also be taken into account, but it will be neglected in our calculation. The main difference with earlier calculations, e.g. the one by Dawson and Oberman[2], lies in the treatment of strong coupling. Our calculation takes accurate account of
the equilibrium electron-ion structure, as well as of full electron-ion dynamics, but it neglects interference effects between ions.

The plasma is assumed to be globally uniform, and confined to volume $\Omega$ with $N$ mobile electrons and $N_i$ ions of charge $Ze$, satisfying charge neutrality $N = ZN_i$. The effect of the ions and a neutralizing uniform background is incorporated in a potential $\Phi(r)$ acting on the electrons, and depending parametrically on the ion positions. The electrostatic potential $\phi(r, t)$ is determined by the electrons and a neutralizing uniform background compensating the one of the ions. The single electron Hamiltonian is therefore given by

$$H(r, p, t) = \frac{p^2}{2m} + \Phi(r) - e\phi(r, t) + eE(t) \cdot r$$  \hspace{1cm} (2)

with Coulomb potential $\phi$ determined by Poisson’s equation

$$\nabla^2 \phi = -4\pi[\rho_{el} + n_0e]$$  \hspace{1cm} (3)

with electron charge density

$$\rho_{el} = -e \int f(r, p, t) dp,$$  \hspace{1cm} (4)

and uniform background density $n_0 = N/\Omega$. The Coulomb potential is therefore

$$\phi(r, t) = \int_{\Omega} \rho_{el}(r', t) + n_0e \frac{1}{|r - r'|} dr'. $$  \hspace{1cm} (5)

The Vlasov-equation for the one-electron distribution function $f(r, p, t)$ reads

$$\frac{\partial f}{\partial t} + \frac{p}{m} \cdot \frac{\partial f}{\partial r} + F \cdot \frac{\partial f}{\partial p} = eE(t) \cdot \frac{\partial f}{\partial p} $$  \hspace{1cm} (6)

with force

$$F = -\frac{\partial \Phi}{\partial r} + e \frac{\partial \phi}{\partial r}. $$  \hspace{1cm} (7)

For vanishing applied field $E(t) = 0$ the Vlasov equation has time-independent solutions of the form $f_0(H_0)$ with time-independent Hamiltonian

$$H_0(r, p) = \frac{p^2}{2m} + \Phi(r) - e\phi_0(r), $$  \hspace{1cm} (8)

with potential $\phi_0(r; R_1, ..., R_{N_i})$ that depends parametrically on the ion positions. Thus in principle many-body effects in the static electron-ion structure are taken into account. In a statistical mechanical theory the structure can be decomposed into 1-ion, 2-ion, 3-ion, etc. effects.

2. Linear response theory

In linear response theory the effect of the applied electric field on the electron distribution is calculated to first order in the field. The calculation leads to an expression for the friction tensor that is exact, but formal, since it still depends on the ion configuration. Finally an average must be performed over the ion distribution function $W(R_1, ..., R_{N_i})$, and at that stage approximations must be made.

In linear response theory the distribution function is expanded in the applied field as

$$f(r, p, t) = f_0(H_0) + f_1(r, p, t) + O(E^2), $$  \hspace{1cm} (9)
where \( f_1(r, p, t) \) is linear in \( E \). It satisfies the equation

\[
\frac{\partial f_1}{\partial t} + \mathcal{L} f_1 = e E \cdot \frac{\partial f_0}{\partial p}
\]  

(10)

with linear evolution operator \( \mathcal{L} \) given by

\[
\mathcal{L} = \mathcal{L}_0 + \mathcal{V},
\]

(11)

where \( \mathcal{L}_0 \) is the single electron Liouville operator corresponding to \( H_0 \)

\[
\mathcal{L}_0 A = \{ A, H_0 \} = \frac{p}{m} \frac{\partial A}{\partial r} + \mathcal{F}_0 \cdot \frac{\partial A}{\partial p},
\]

(12)

and the linear operator \( \mathcal{V} \) is defined by

\[
\mathcal{V} A = -e^2 f'_0 \frac{p}{m} \cdot \frac{\partial}{\partial r} \int_{\Omega} \int \frac{1}{|r - r'|} A(r', p') \, dr' dp',
\]

(13)

where \( f'_0 = df_0/dH_0 \). For harmonic oscillating field \( E(t) = E_0 \exp(-i\omega t) \) we consider the solution of Eq. (10) oscillating with the same time-factor

\[
(-i\omega + \mathcal{L}) f_1 = \frac{e}{m} E_0 \cdot \mathcal{F}_0.
\]

(14)

The formal solution is

\[
f_1 = \frac{e}{m} (-i\omega + \mathcal{L})^{-1} E_0 \cdot \mathcal{F}_0.
\]

(15)

We are interested in the mean electron velocity \( V(t) \). In the stationary state \( V_0 = 0 \), by symmetry in the momentum. To first order in \( E_0 \), with omission of the exponential time-factor,

\[
V_1 = \frac{1}{N} \int_{\Omega} \int \frac{p}{m} f_1(r, p) \, dr dp.
\]

(16)

Substituting from Eq. (15) we find that the first order mean velocity is given by

\[
V_1 = -e \mathcal{Y} \cdot E_0
\]

(17)

with admittance tensor

\[
\mathcal{Y}(\omega, X, \Omega) = \frac{-1}{Nm^2} \int_{\Omega} \int p(-i\omega + \mathcal{L})^{-1} f'_0 \, dr dp.
\]

(18)

The tensor depends parametrically on the configuration \( X = (R_1, ..., R_N) \) of ions. We must average over the probability distribution of configurations to get the conductivity. Note that the admittance tensor \( \mathcal{Y}(\omega, X, \Omega) \) is the Fourier transform of an electron velocity time-correlation function for fixed ion configuration.

By formal manipulation[1] the admittance tensor can be put in the form

\[
\mathcal{Y}(\omega, X, \Omega) = [ -i\omega m 1 + \zeta(\omega, X, \Omega)]^{-1}
\]

(19)

with friction tensor \( \zeta(\omega, X, \Omega) \) given by

\[
\zeta(\omega, X, \Omega) = \zeta_0(\omega, X, \Omega)[1 + A_{Fv}(\omega, X, \Omega)]^{-1}
\]

(20)
with tensors $A_{Fv}$ and $\zeta_i$ given by

$$A_{Fv}(\omega, X, \Omega) = \frac{-1}{Nm} \int_\Omega \int \mathcal{F}_b \xi p f_0' \, dr dp,$$

$$\zeta_i(\omega, X, \Omega) = \frac{-1}{N} \int_\Omega \int \mathcal{F}_b \mathcal{F}_0 f_0' \, dr dp,$$  \hspace{1cm} (21)

with bare force $\mathcal{F}_b$ and screened force $\mathcal{F}_0$ given by

$$\mathcal{F}_b = -\frac{\partial \Phi}{\partial r}, \quad \mathcal{F}_0 = \mathcal{F}_b + e\frac{\partial \phi_0}{\partial r}. \hspace{1cm} (22)$$

After averaging over ion configurations one can apply a cluster expansion. In the low density limit the tensor $A_{Fv}$ can be neglected, and the problem can be reduced to the calculation of a single-ion friction coefficient.

**3. Single-ion friction coefficient**

For a disordered system of ions we can average the exact relations derived above over the probability distribution of configurations $W(X)$, assumed given. The system is assumed to become uniform and isotropic in the thermodynamic limit. Then by the same arguments as for a system of independent electrons[3] we arrive for low density of ions at the expression for the friction coefficient

$$\zeta_1(\omega) = -\frac{1}{3} n_i \int \int \mathcal{F}_b(r) \cdot G(1) \mathcal{F}_0(r) \phi_0(\varepsilon) \, dr dp,$$  \hspace{1cm} (23)

where $n_i$ is the density of ions, and $\phi_0'(\varepsilon)$ is the derivative with respect to energy $\varepsilon$ of the stationary electron distribution $\phi_0(\varepsilon)$, normalized such that

$$\int \phi_0(H_0(1)) dp \to 1 \quad \text{as} \quad r \to \infty. \hspace{1cm} (24)$$

Here $\varepsilon$ is the value of the Hamiltonian

$$H_0(r, p; 1) = \frac{p^2}{2m} + v_0(r), \quad v_0(r) = v_b(r) - e\phi_0(r) \hspace{1cm} (25)$$

for an electron with a single ion centered at the origin. The bare ion potential $v_b(r)$ is centrally symmetric and has long-range part $-Ze^2/r$. It is screened by the potential $-e\phi_0(r)$. The bare force $\mathcal{F}_b(r)$ in Eq. (23) is simply the gradient $-\partial v_b/\partial r$, and the operator $G(1)$ is the inverse $(-i\omega + \mathcal{L}(1))^{-1}$ with evolution operator $\mathcal{L}(1)$ for the linearized Vlasov equation corresponding to the equilibrium distribution

$$f_0(r, p) = n_0^{(0)} \phi_0(H_0(1)), \hspace{1cm} (26)$$

where $n_0^{(0)}$ is the asymptotic free electron density. The potential $\phi_0(r)$ must be found self-consistently from the solution of Poisson’s equation

$$\nabla^2 \phi_0 = 4\pi e \left[ \int f_0(r, p) \, dp - n_0^{(0)} \right]. \hspace{1cm} (27)$$

In practical applications the distribution $f_0(r, p)$ will be a Maxwell-Boltzmann or Fermi-Dirac distribution. The force $\mathcal{F}_0(r)$ in Eq. (23) is given by

$$\mathcal{F}_0(r) = -\frac{\partial \phi_0}{\partial r} = \mathcal{F}_b(r) + e\frac{\partial \phi_0}{\partial r}. \hspace{1cm} (28)$$
In the limit of zero electron charge the expression (23) for the friction coefficient reduces to that found for the Lorentz-model[3]. The electrical conductivity corresponding to the frequency-dependent friction coefficient in Eq. (23) is found by substitution into Eq. (1). The subscript 1 indicates that only a single scatterer is involved in the calculation of the friction coefficient. In principle interference effects between two ions may be considered. This would involve a study of the pair contribution in the cluster expansion.

In order to evaluate the single-ion friction coefficient $\zeta_1(\omega)$ given by Eq. (23) we must solve a linearized Vlasov equation in the presence of the screened ion potential $v_0(r)$, namely

$$-i\omega f_{1\alpha} + \frac{p}{m} \cdot \frac{\partial f_{1\alpha}}{\partial r} + F_0(r) \cdot \frac{\partial f_{1\alpha}}{\partial p} - eE_{1\alpha}(r) \cdot \frac{\partial f_0}{\partial p} = F_{0\alpha}(r)\varphi'_0(r, p)$$  \hspace{1cm} (29)

with first order electric field $E_{1\alpha}(r)$ given by

$$E_{1\alpha}(r) = e \frac{\partial}{\partial r} \int \int \frac{1}{r - r'} f_{1\alpha}(r', p') \, dr' dp'$$  \hspace{1cm} (30)

for each of the three cartesian components $\alpha = (x, y, z)$. The friction coefficient follows from the solution as

$$\zeta_1(\omega) = -\frac{1}{3n_i} \int F_b(r) \cdot f_1(r, p, \omega) \, dr dp.$$  \hspace{1cm} (31)

It is worthwhile to consider the exact high-frequency behavior of the friction coefficient that follows from these expressions. This is given by

$$\zeta_1(\omega) = \frac{1}{3i\omega n_i} \int F_b(r) \cdot F_0(r)\varphi'_0(r, p) \, dr dp + O(1/\omega^2).$$  \hspace{1cm} (32)

For an ion with a point nucleus with charge $Z_p e$ the bare potential $v_b(r)$ diverges at short distance as $-Z_p e^2/r$, and so does the shielded potential $v_0(r)$. Since the potential is attractive the distribution $\varphi_0(r, p)$ makes the short-distance singularity even worse. For such a potential the short-time coefficient in Eq. (32) diverges. For attractive force the classical model considered here can handle only soft pseudopotentials without point nucleus. The pseudopotential must follow from a separate quantummecanical calculation.

We have solved the set of equations explicitly[1] for a particular choice of the bare ion pseudopotential $v_b(r)$. In order to simplify the calculation we have restricted attention to a Fermi-Dirac distribution at $T = 0$ for $\varphi_0(\varepsilon)$, so that its derivative with respect to $\varepsilon$ is proportional to a delta-function at Fermi-energy $\varepsilon_0$. By use of central symmetry the six-dimensional integration over $dr dp$ in Eq. (31) can be reduced to a three-dimensional integration over $dr dp d\xi$, where $\xi = \hat{r} \cdot \hat{p}$ is the cosine of the angle between $r$ and $p$. We can transform to variables $(\varepsilon, \lambda, s)$, where $\varepsilon$ is the energy, $\lambda$ is the angular momentum, and $s$ is a time-like running variable along the orbit $(\varepsilon, \lambda)$. In the transformation the volume-element transforms as

$$2r^2 p^2 dr dp d\xi = d\varepsilon d\lambda^2 ds.$$  \hspace{1cm} (33)

By the choice of $\varphi_0(\varepsilon)$ the integration over $\varepsilon$ restricts the energy to value $\varepsilon_0$, and we are left with a two-dimensional integral. Before sketching the details of the calculation, we relate the expression (23) for the single-ion friction coefficient to earlier work.

4. Relation to Boltzmann equation and dielectric theory

In the absence of the self-consistent field, i.e. in the case of non-interacting electrons, we have $F_0 = F_b$, and the expression (3.1) reduces to

$$\zeta_{1b}(\omega) = -\frac{1}{3n_i} \int F_b(r) \cdot G(1) F_b(r)\varphi'_0(\varepsilon) \, dr dp.$$  \hspace{1cm} (34)
This leads to a frequency-dependent generalization of the Lorentz-model[3]. In other words, it amounts to a generalization of the Boltzmann equation to non-markovian effects. In the limit of zero frequency there must therefore be a relation to the original Lorentz-model. In fact one has for a step-function in energy

$$\varphi_0(\varepsilon) = A\theta(\varepsilon_0 - \varepsilon), \quad A = \frac{3}{4\pi}(2m\varepsilon_0)^{-3/2},$$  \hspace{1cm} (35)

where the normalization constant $A$ follows from Eq. (24), the relation[3]

$$\zeta_1b(0) = n_i\sqrt{2m\varepsilon_0}\sigma_1(\varepsilon_0),$$  \hspace{1cm} (36)

where

$$\sigma_1(\varepsilon_0) = 2\pi \int (1 - \cos \chi) b \, db$$  \hspace{1cm} (37)

is the transport cross section for collisions with scattering angle $\chi$ at energy $\varepsilon_0$ and impact parameter $b$.

More generally, at any frequency Eq. (34) can be written as

$$\zeta_1b(\omega) = -\frac{4\pi^2}{3} n_i \int \hat{C}_+(\omega; \varepsilon)\varphi_0'(\varepsilon) \, d\varepsilon,$$  \hspace{1cm} (38)

where the function $\hat{C}_+(\omega; \varepsilon)$ can be decomposed into an integral of contributions from different angular momenta

$$\hat{C}_+(\omega; \varepsilon) = \int \hat{C}_+(\omega; \varepsilon, \lambda) \, d\lambda^2.$$  \hspace{1cm} (39)

The integrand in the last expression can be written as the one-sided Fourier transform of a time-correlation function

$$\hat{C}_+(\omega; \varepsilon, \lambda) = \int_0^\infty e^{i\omega t} C(t; \varepsilon, \lambda) \, dt.$$  \hspace{1cm} (40)

The time-correlation function

$$C(t; \varepsilon, \lambda) = \int_{-\infty}^{\infty} F_b(r) F_b'(r, t) \, ds$$  \hspace{1cm} (41)

is calculated as an integral along the orbit $(\varepsilon, \lambda)$. One can show[4]

$$\hat{C}_+(0; \varepsilon) = \frac{4}{\pi} m^2 \varepsilon^2 \sigma_1(\varepsilon),$$  \hspace{1cm} (42)

and this establishes the relation (36) to the scattering cross section. It is straightforward to calculate the frequency-dependent friction coefficient from Eqs. (38–41), as demonstrated recently for the case of repulsive power law potentials[5].

The expression for the dynamical friction coefficient derived in the preceding section is closely related to approximate expressions derived for the energy loss of a charged particle moving through an electron gas, in terms of the dielectric function $\epsilon(k, \omega)$ of the uniform plasma. The theory is sometimes known as the dielectric theory. Excellent reviews of energy-loss theory have been presented by Pines and Nozières[7], by Calkin and Nicholson[8], and by Gerlach and Grosse[9][20]. Similar approximate results have been derived in the theory of conductivity in the work of Dawson and Oberman[2], Perel’ and Eliashberg[11], Ron and Tzoar[12], and Götze and Wölfle[13]. The last three papers are based on quantum mechanics.
The approximate result of energy-loss theory may be expressed in terms of the friction coefficient as

\[ \zeta^{(e)}(\omega) = \frac{2\pi^2 i}{3Ze^2 \omega} \int k^4 |\hat{\nu}_b(k)|^2 \left( \frac{1}{\epsilon(k,\omega)} - \frac{1}{\epsilon(k,0)} \right) dk, \]  

(43)

where \( \hat{\nu}_b(k) \) is defined by

\[ \hat{\nu}_b(k) = \frac{1}{8\pi^3} \int \exp[-ik \cdot r] \nu_b(r) \, dr, \]  

(44)

and where \( \epsilon(k,\omega) \) is the dielectric function of the uniform electron gas with distribution \( \varphi_0^{(0)}(p) \) given by

\[ \epsilon(k,\omega) = 1 + \frac{\omega_p^2}{k^2} \int \frac{k \cdot p}{\omega - k \cdot p/m} \varphi_0^{(0)}(p) \, dp, \]  

(45)

with plasma frequency

\[ \omega_p = \sqrt{\frac{4\pi n_0^{(0)} e^2}{m}}. \]  

(46)

In particular, the expression of Dawson and Oberman\[2\] for a classical plasma with bare potential \( \nu_b(r) = -Ze^2/r \) reads

\[ \zeta^{(e)}(\omega) = \frac{2i\pi}{3\epsilon^{(0)} } \int_0^{k_{\text{max}}} \frac{k^2}{\omega} \frac{1}{\epsilon(k,\omega)} - \frac{1}{\epsilon(k,0)} \frac{k^2 \Phi(k,\omega)}{\epsilon(k,\omega)} \, dk. \]  

(47)

Here a wavenumber cutoff \( k_{\text{max}} \) is required, because of the point singularity in the potential, and \( \epsilon(k,\omega) \) is the dielectric function of the uniform electron gas with Maxwell-Boltzmann distribution at temperature \( T \).

We can obtain this expression from our theory by making two approximations:

1. Replace the linearized Vlasov equation with central potential (3.7) by

\[ -i\omega f_{1\alpha} + \frac{P}{m} \frac{\partial f_{1\alpha}}{\partial r} - eE_{1\alpha}(r) \cdot \frac{\partial f_{0\alpha}^{(0)}}{\partial p} = F_{0\alpha}(r)\varphi_0^{(0)}(p), \]  

(48)

i.e. use the uniform distribution \( f_{0\alpha}(p) \simeq \varphi_0^{(0)}(p) \) and drop the ion force \( F_{0\alpha}(r) \) on the left-hand side of the equation. This yields the approximate expression

\[ \zeta_{11}^{(e)}(\omega) = -\frac{8\pi^3 i}{3} \int \hat{F}_{0k} \cdot \hat{F}_{0k} \frac{\Phi(k,\omega)}{\epsilon(k,\omega)} \, dk \]  

(49)

with the abbreviation

\[ \Phi(k,\omega) = \int \frac{\varphi_0^{(0)}(p)}{\omega - k \cdot p/m} \, dp = \frac{k^2}{m\omega_p^2} [\epsilon(k,\omega) - \epsilon(k,0)]. \]  

(50)

2. Replace the Fourier transform of the shielded force \( F_{0\alpha}(r) \) by

\[ \hat{F}_{0k}^{(0)} = \hat{F}_{0k}/\epsilon(k,0). \]  

(51)

Dawson and Oberman\[2\] assume the Maxwell-distribution for the unperturbed electron gas, but that is not an essential feature of their theory. Our calculation improves on the one of Dawson and Oberman by use of the complete equilibrium electron-ion structure \( \varphi_0(r,p) = \varphi_0(\epsilon) \), and complete dynamics of electrons in the central ion potential with interactions between electrons described in Vlasov approximation.
5. Explicit calculation

Both the exact and approximate theories take account of screening, so that there is no long range (or small \(k\)) divergence. However, both theories give divergence at short distance (or large \(k\)) for a point ion with bare potential

\[
v_b(r) = -\frac{Ze^2}{r}. \tag{52}
\]

The divergence is actually worse in the exact theory, since the attractive potential leads to an increased density of electrons at short distance. The short-range divergence of the classical theory can be resolved properly only in a fully quantummechanical theory. Quantummechanical treatments in weak-coupling or Born approximation have been proposed by Bornath et al.\[13\], and by Kull and Plagne\[14\].

We have studied strong coupling effects in the framework of the classical theory, taking quantummechanical diffraction effects into account in terms of a pseudopotential\[15\] \(v_b(r)\) that is finite for \(r \to 0\). In particular we use a bare pseudopotential of the form

\[
v_b(r) = -\frac{Ze^2}{r}(1 - e^{-\alpha r}). \tag{53}
\]

From Poisson’s equation one calculates the equivalent bare charge density as

\[
\rho_b(r) = \frac{Ze^2}{4\pi\alpha^2} \frac{e^{-\alpha r}}{r}. \tag{54}
\]

A potential of the form (53) with \(\alpha = 1/\lambda_{deB}\), where \(\lambda_{deB}\) is the thermal de Broglie wavelength was proposed by Deutsch et al.\[16\],\[17\],\[18\], and used in molecular dynamics simulation of a 2-component plasma by Hansen and McDonald\[19\].

As argued at the end of Sec. 3, in numerical calculation it is advantageous to limit attention to electron orbits of a single energy \(\varepsilon_0\). In the expression (23) for the friction coefficient we need the derivative \(\varphi'_0(\varepsilon) = d\varphi_0(\varepsilon)/d\varepsilon\), so that we can use a Fermi-Dirac distribution at temperature \(T = 0\) with Fermi-energy \(\varepsilon_0\).

In our numerical calculation we use in particular

\[
\varepsilon_0 = \frac{e^2}{2a_0}, \tag{55}
\]

with Bohr radius \(a_0 = \hbar^2/me^2\). With \(\varepsilon_0 = k_B T_0\) this corresponds to a temperature \(T_0 = 1.5 \times 10^6\) °K. The density \(n_0(0) = (8\pi/3h^3)(2m\varepsilon_0)^{3/2}\), with mean interparticle distance \(r_0\) defined by \(4\pi n_0(0) r_0^3 = 1\), corresponds to a ratio \(r_s = r_0/a_0 = 1.9\), slightly less than for most metals at normal pressure\[6\]. For \(r_s << 1\), i.e. high density of electrons, the system properties are supposed to be well described by the random phase approximation\[6\], i.e. by dielectric theory. We have determined the parameter \(\alpha\) in the pseudopotential, given by Eq. (53), from the exact quantummechanical condition\[20\]

\[
\left.\frac{dn_0}{dr}\right|_{r=0} = -\frac{2Z}{a_0} n_0(0). \tag{56}
\]

A Thomas-Fermi calculation\[1\] yields \(\alpha = 2.3/a_0\).

The calculation of the friction coefficient \(\zeta_1(\omega)\), given by Eq. (23), proceeds as indicated in Eqs.(38–41), but with time-correlation function

\[
C(t; \varepsilon, \lambda) = \int_{-\infty}^{\infty} F_b(r) F_b(r,t) \, ds, \tag{57}
\]
where the integration is along the orbit \((\varepsilon, \lambda)\) for the screened potential \(v_0(r)\). Thus \(r(s, \varepsilon, \lambda)\) in the first factor is found from integration of the orbit equation

\[
\frac{dr}{ds} = \sqrt{\frac{2}{m}} \left[ \varepsilon - v_0(r) - \frac{\lambda^2}{2mr^2} \right]^{1/2}.
\]  

(58)

The time-dependence of the second factor \(F_0(r, t)\) follows from the solution of a linearized Vlasov-equation with self-consistent potential calculated at each time-step by integration over \((\varepsilon', \lambda', s')\). The time-dependent force on the orbit \((\varepsilon, \lambda)\) may be expressed as

\[
F_0(r, t) = r g(s, t) + \xi ph(s, t),
\]

(59)

with radial momentum \(p(s, \varepsilon, \lambda)\) given by

\[
p = \sqrt{2m[\varepsilon - v_0(r)]},
\]

(60)

and with angular variable \(\xi(s, \varepsilon, \lambda)\) given by

\[
\xi = \pm \sqrt{1 - \frac{\lambda^2}{2mr^2p^2}}.
\]

(61)

The linearized Vlasov-equation may be shown to be equivalent to the two coupled equations

\[
\begin{align*}
\frac{\partial g}{\partial t} + \frac{\partial g}{\partial s} + \frac{F_0(r)}{r} h &= \frac{\partial T}{\partial s}, \\
\frac{\partial h}{\partial t} + \frac{\partial h}{\partial s} + \frac{1}{m} g &= \frac{1}{m} T,
\end{align*}
\]

(62)

for orbit \((\varepsilon, \lambda)\) with \(T\) given by an integral linear in \(g(s', t, \varepsilon', \lambda')\) and \(h(s', t, \varepsilon', \lambda')\). The time-correlation function \(C(t; \varepsilon, \lambda)\) in Eq. (57) must be calculated numerically for a sufficient number of sufficiently small time-steps.

6. Numerical results

In our numerical work we have studied the example discussed in the preceding section. We have calculated the single-ion friction coefficient \(\zeta_1(\omega)\), given by Eq. (23), and have compared with the approximate friction coefficient of the dielectric theory \(\zeta_1^{(0)}(\omega)\), given by Eq. (43), and with the friction coefficient of the dielectric theory with improved screening \(\zeta_1^{(0)}(\omega)\), given by Eq. (49). In all three cases the calculation was performed for the same pseudopotential. In Fig. 1 we compare the bare pseudopotential \(v_0(r)\) in atomic units with the corresponding screened potential \(v_0(r)\). In Fig. 2 we compare their Fourier transforms.
We have seen in Eq. (32) that at high frequency the friction coefficient behaves as

\[ \zeta_1(\omega) \approx \frac{A_1}{-i\omega}. \]  

The coefficient \( A_1 \) follows from the initial value \( C(0; \varepsilon_0) \). This may be evaluated by quadrature from

\[ C(0; \varepsilon) = \int_0^\infty \int_{-\infty}^{\infty} F_b(r(s; \varepsilon, \lambda))F_0(r(s; \varepsilon, \lambda)) \, d\lambda \, ds. \]  

The corresponding value of the coefficient in the dielectric theory is

\[ A_1^{(\varepsilon)} = \frac{8\pi^3}{3Ze^2}\kappa^2 \int_0^\infty |\hat{v}_b(k)|^2 \frac{k^6}{k^2+\kappa^2} \, dk, \]  

with inverse screening length \( \kappa \), and in the dielectric theory with improved screening

\[ A_1^{(0)} = \frac{8\pi^3}{3Ze^2}\kappa^2 \int_0^\infty \hat{v}_b(k)^*\hat{v}_0(k)k^4 \, dk. \]  

The numerical values in our example are for \( Z = 1 \) in atomic units

\[ A_1 = 0.276, \quad A_1^{(\varepsilon)} = 0.220, \quad A_1^{(0)} = 0.208. \]  

At zero frequency we find from the three calculations

\[ \zeta_1(0) = 0.081, \quad \zeta_1^{(\varepsilon)}(0) = 0.121, \quad \zeta_1^{(0)}(0) = 0.114. \]
This shows that for the model considered the three calculations yield appreciably different results.

In Fig. 3 we plot the real part of the friction coefficient $\Re \zeta_1^{(0)}(ω)$, as calculated from Eq. (49) for the model discussed above, as a function of frequency, and compare with $\Re \zeta_1^{(e)}(ω)$, as calculated from Eq. (43). There is a pronounced resonance starting at the plasma frequency, corresponding to emission of plasma waves.

In Fig. 4 we plot the time-correlation function $C(t; ε_0)$, as calculated by the numerical procedure indicated in Sec. 5. In Fig. 5 we plot the real part of the friction coefficient $\Re \zeta_1(ω)$ as a function of frequency and compare with the approximate $\Re \zeta_1^{(0)}(ω)$, as calculated from Eq. (49). Again there is a pronounced resonance at the plasma frequency, but the discontinuity in slope of the approximate theory is eliminated.
7. Discussion
We have shown in the framework of the Lorentz-Vlasov model of a classical plasma that the interaction of a selected ion with the mobile electrons can be fully taken into account. The calculation shows that for the chosen example the frequency-dependence of the friction coefficient differs significantly from that found from dielectric or energy-loss theory. In other words, the frequency spectrum of inverse bremsstrahlung depends on the details of the electron-ion dynamics, and the impact or Born approximation is poor if the electron-ion coupling is strong. An accurate account of the frequency-dependence requires a fairly elaborate calculation.

In our theory the interaction between electrons has been treated in Vlasov-approximation. In earlier work by Cauble and Rozmus[21] an attempt was made to incorporate correlations between electrons. These authors also found significant deviations from the prediction of the dielectric theory. It would be of interest to compare with their theory in detail for the model studied here.

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