

Electric field dynamics at charged point in two component plasma

M.T. Meftah^{1,a}, T. Chohra¹, H. Bouguettaia¹, F. Khelfaoui¹, B. Talin², A. Calisti², and J.W. Dufty³

¹ Laboratoire des Énergies Nouvelles et Renouvelables dans les Zones Arides et Sahariennes Lenreza, Université de Ouargla 30000, Algeria

² Laboratoire des Interactions Ioniques et Moléculaires PIIM, service 232 Centre Saint-Jérôme, 13397 Marseille, France

³ Department of Physics, University of Florida, Gainesville, Florida 32611, USA

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Abstract. The autocorrelation function for the velocity and for the electric microfield of an impurity ion in a Two Ionic Component Plasma (TICP) is considered. A simple model is constructed for this purpose that preserves the exact short time dynamics and the long time global constraint of a given self-diffusion coefficient. The memory function and then the collision effects associated with the correlation function for the self-diffusion are expressed in terms of an effective two body interaction via a screened effective potential. The basic approximation used in our approach is the “disconnected” one that refers to the collision operator. A comparison of the prediction of this model for the self-diffusion and for the autocorrelation functions with the results of the molecular dynamics simulation developed in our laboratory (PIIM) shows an acceptable agreement over a wide range of plasma coupling, impurity ion charge and concentration.

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1 Introduction

In the last decade very little progress, despite a certain number of unexpected features, has been made for the dynamics properties of the electric field at a neutral point in a plasma [2–7]. In contrast, the probability distribution for a given value of the microfield in an equilibrium plasma is a well-studied problem with an accurate precision.

Our aim in this work is to extend the earlier studies of the electric field dynamics to the case of charged impurity ions embedded in TICP itself in neutralizing a background of negative charges. The reason for this choice is that, in the general case, the plasma is constituted of many ionic species. The presence of the charged ion in the plasma changes the physics of the problem with respect to the neutral point because the presence of the ion significantly changes the charge distribution of the plasma in its vicinity.

Our model is based on the most important symmetries of the correlation function and the relationship with the structure and the transport properties. For example, the time integral of $C(t)$ must vanish exactly as a consequence of the field being proportional to the total force on the

ion impurity. For similar reasons, there is a simple and exact relationship between the ion velocity autocorrelation function, $D(t) = \langle \vec{V}(t)\vec{V} \rangle / \langle V^2 \rangle$ and the self diffusion coefficient D through an exact Green-Kubo formula.

The model is then constructed from an exact master equation for $D(t)$ describing the linear response of the impurity ion to an initial perturbation of its velocity, and it provides a clear interpretation of the dynamics as damped oscillatory motion in a viscoelastic medium. The complex many-body dynamics is represented in our model by a memory function which is approximated by a simple exponential time relaxation. The time scale for this relaxation is fixed by the above-mentioned Green-Kubo formula. The only input required in our model is the initial values of the autocorrelation function, its derivatives and the self-diffusion coefficient D . These are calculated using the “disconnected approximation” [9] for the self-diffusion coefficient and the HNC equation [8] for the pair correlation (static structure functions). As a result, the two dynamic properties $D(t)$ and $C(t)$ obeying linear equations may be expressed as functions of the self-coefficient D and the initial data. None of these approximations implies a priori any limitation with respect to the plasma coupling strength, ion charge, ion mass or time scale. Consequently,

^a e-mail: meftah@ouargla-univ.dz

the model could be considered as a good candidate for the description of electric field dynamics over a wide range of conditions.

The time dependence of this model can be expressed as a linear combination of three exponentials or modes, allowing a simple interpretation of the relevant plasma excitations responsible for the electric field dynamics. At a weak coupling, all three modes represent purely damped excitations, while at strong coupling there is one damped mode and a complex conjugate pair of damped propagating modes. The conditions of “weak” or “strong” coupling depend on the plasma coupling, charge, mass and the concentrations of the two components. To limit the parameters space, we consider the simplest case of the TICP with the same sign ions which differ in their charge number in the classical limit. The relevant parameters are then the TICP coupling constant $\Gamma = \beta q_0^2/a_s$, the charge ratio q_0/q , and the mass ratio m_0/m , where a_s is the ion sphere radius, $\beta = 1/k_\beta T$, and parameters with the subscript 0 refer to the impurity ion. We have considered here the TICP with the screened interaction.

The approximation described here for $C(t)$ is a special investigation of an earlier work which calculated the effects of ion motion on spectral line broadening in plasma [8,9]. The aim of the present work is then to isolate, via a Zwanzig projection formalism, the simplest features of the electric field dynamics from the complexities of the general context. This leads to a clear interpretation, analysis and a comparison with computer simulations.

2 The model

The system considered here is an embedded impurity ion of mass m_0 and charge q_0 in an equilibrium with a fully ionized plasma of structureless point ions. The plasma is composed of two ionic species. One of them has the same properties (m_0, q_0) as the embedded impurity whereas the other is different (mass m and charge q). We have to deal with this model because it is close to a realistic system since in the plasma, at least, one ionic component (species) is present. The electric field at the impurity ion due to the rest of plasma is given by:

$$\vec{E} = \sum_{\alpha} \sum_{i=1}^{N_{\alpha}} \vec{e}_{\alpha}(\vec{r}_i - \vec{r}_0) + \vec{E}_B \quad (1)$$

where N_{α} is the number of ions of species α , $\vec{e}_{\alpha}(\vec{r}_i - \vec{r}_0)$ is the field due to the plasma ion at a distance $|\vec{r}_i - \vec{r}_0|$ from the impurity ion and \vec{E}_B is the field due to the uniform neutralizing background charge. The equilibrium autocorrelation function of the electric field is defined by:

$$C(t) = \left\langle \vec{E}(t) \vec{E} \right\rangle / \langle E^2 \rangle \quad (2)$$

where the brackets $\langle \dots \rangle$ denote an equilibrium Gibbs ensemble average. As denoted in the introduction, this function plays a central role in many theories of radiative and

transport processes in plasmas. A closely related function for transport properties is the velocity autocorrelation:

$$D(t) = \left\langle \vec{V}_0(t) \cdot \vec{V}_0 \right\rangle / \langle V_0^2 \rangle \quad (3)$$

where \vec{V}_0 is the velocity of the impurity ion. The autocorrelation function $C(t)$ measures the fluctuations in a collective property of the TICP while $D(t)$ measures fluctuations in a property of the impurity ion. However, these are directly related by Newton’s first law

$$\frac{\partial^2 D(t)}{\partial t^2} = -\omega_0^2 C(t), \quad \omega_0^2 = (\beta q_0^2/3m_0) \langle E^2 \rangle. \quad (4)$$

The interpretation of our model is more direct in terms of $D(t)$. First, a formally exact equation is derived by using the Zwanzig projection operator (see Appendix A.1):

$$\frac{\partial^2 D(t)}{\partial t^2} + \omega_0^2 D(t) + \int_0^t d\tau M(t-\tau) \frac{\partial D(\tau)}{\partial \tau} = 0 \quad (5)$$

$$M(0) = \omega_1^2 - \omega_0^2, \quad \omega_1^2 = \left\langle \dot{E}^2 \right\rangle / \langle E^2 \rangle \quad (6)$$

where \dot{E} indicates the time derivative of the microfield $\vec{E}(t)$ at $t = 0$. Equation (5) describes the impurity ion dynamics as oscillations in a viscoelastic medium with the characteristic frequency ω_0 and shows a frequency dependent damping given by the Laplace transform of $M(t)$. All many-body effects of the medium on the impurity that are not explicit in (5) are contained in the detailed form of $M(t)$ [6]. Our fundamental assumption here, is that, it is sufficient to include only the magnitude of this function through its exact initial value $M(0)$ and a characteristic time scale of its decay [6]. Consequently, $M(t)$ is approximated by:

$$M(t) = M(0)e^{-\lambda t}. \quad (7)$$

The precise form of λ is fixed by the Green-Kubo expression for the self diffusion coefficient, D , in terms of the velocity autocorrelation function as [6]:

$$\beta m_0 D = \int_0^{\infty} dt D(t). \quad (8)$$

The use of (5) with (7) in order to determine the right hand side of (8), leads to the identification:

$$\lambda = (\omega_1^2/\omega_0^2 - 1) / (\beta m_0 D). \quad (9)$$

Equations (5–7) and (9) define the approximate model for $D(t)$ and through (4), the electric field autocorrelation function. Furthermore, the exact time integrals of $C(t)$ and $D(t)$ are assured through (4) and (8). The input data ω_0 , ω_1 , and D might be taken directly from a computer simulation. Alternatively, as will be discussed below, additional independent approximations may be introduced to allow a practical calculation of these parameters.

The choice of (q_0/q) , (m_0/m) , Γ and (n_1/n_2) will determine whether the solutions are a pair of oscillatory

functions (under-damped), or three real exponential functions (over-damped). More generally, if λ/ω_0 is not large, the medium exhibits “memory” and the damping is modified on time scales of the order of λ^{-1} . Thus, there are only four parameters that completely characterize the dynamics of the model ω_0 , ω_1 , λ and the ratio (n_1/n_2) . It is therefore, straightforward to solve (5) by Laplace transform, yielding $D(t)$ and $C(t)$ as the sum of three exponentials:

$$D(t) = \sum D_i e^{z_i t}, C(t) = \sum C_i e^{z_i t} \quad (10)$$

where the coefficients D_i and C_i are given by:

$$D_i = -(\omega_0/z_i)^2 C_i \quad (11)$$

$$C_1 = (\lambda + z_1) z_1 (z_3 - z_2) / \Delta \quad C_2 = (\lambda + z_2) z_2 (z_1 - z_3) / \Delta \quad (12)$$

$$C_3 = (\lambda + z_3) z_3 (z_2 - z_1) / \Delta \quad \Delta = (z_1 - z_2)(z_2 - z_3)(z_3 - z_1) \quad (13)$$

and the $\{z_i\}$ are solutions to the cubic equation:

$$z^3 + \lambda z^2 + \omega_1^2 z + \lambda \omega_0^2 = 0 \quad (14)$$

depending on the values of λ , ω_0 and ω_1 : the solutions may be either real or complex. This ends the theoretical model description, and to evaluate its predictions it must be compared to the corresponding molecular dynamics simulations (MDS). Such simulations have been used in many areas of physics to provide statistical information, static as well dynamic properties of many physical quantities. A standard MDS is devoted to solve numerically Newton’s Law in a many-body system. It consists of a few hundred particles (ions) interacting via a screened Coulomb potential moving in a cubic box with periodic boundary conditions, maintaining the system in a stationary state at a fixed temperature and density. To accomplish this, it is assumed in MDS that the forces between the ions are conservative, two-body forces, that is, energy is conserved and the total force acting on the ion (the impurity in our case) due to the other ions is the sum of the forces between the pairs of ions. Once the force on the impurity ion is known at the initial time (boundary conditions), the MDS enables us to follow the ion trajectory and to know, at any subsequent time, the impurity velocity $\vec{V}(t)$ and the microfield $\vec{E}(t)$ acting on this impurity. The acknowledgment of these time dependent quantities, $\vec{V}(t)$ and $\vec{E}(t)$, is sufficient to compute the autocorrelation microfield function $C(t) = \langle \vec{E}(t) \vec{E}(0) \rangle$ and the autocorrelation velocity function $D(t) = \langle \vec{V}(t) \vec{V}(0) \rangle$.

The analysis made up to this point applies for arbitrary interaction potentials and plasma composition. To illustrate the physical content of the model, we consider the special case of the TICP with an impurity ion of the same mass and the same charge (m_0, q_0) for one component of the plasma ions. In this case, there is only one dimensionless parameter characterizing the plasma state

Table 1. Diffusion coefficient of Ar^{+17} in $(\text{Ar}^{+17}, \text{He}^{+1})$ with different concentrations.

$\text{Ar}^{+17}\%$	He^{+1}	D_{Ar}^*
25	75	1.8
50	50	2.84
75	25	8.34
90	10	18.61

condition, $\Gamma = q_0^2 \beta / a_s$ with $a_s = (4/3n_i \pi)^{1/3}$ is the average interparticle distance (ion sphere radius) and $n_i = n_1 + n_2$ is an ionic plasma density. Table 1 shows the Γ dependence on ω_0 , ω_1 (in units of the electronic plasma frequency ω_p defined by $\omega_p^2 = 4\pi n_e e^2 / m_e$), and $D_* = D / (a_s^2 \omega_p)$ is evaluated for screened interactions treated in the present paper.

3 Determination of parameters λ , ω_0 , ω_1

We attempt now to determine all the parameters necessary in the description of the dynamics. These parameters allow us, first, to solve the algebraic equation (14) and then to describe the dynamics properties of the ionic mixture. We shall see, as mentioned in the introduction, that these parameters are at first sight directly related to the initial values of the autocorrelation function and its first derivative ($\omega_0^2 \sim C(0) \sim \langle E^2 \rangle$ and $\omega_1^2 \sim \dot{C}(0) \sim \langle \dot{E}^2 \rangle$) and secondly related to the static pair functions like $g_{0\alpha}(r)$.

Consider first ω_0 defined by (4),

$$\omega_0^2 = \left(\frac{\beta q_0^2}{3m_0} \right) \langle E^2 \rangle = - \left(\frac{\beta q_0}{3m_0} \right) \langle \vec{E} \cdot \vec{\nabla}_0 U \rangle \quad (15)$$

where U is the potential energy of the interaction between the impurity ion and the surrounding plasma. This expression (15) can be rewritten, after making a part integral, as:

$$\omega_0^2 = - \left(\frac{q_0}{3m_0} \right) \langle \vec{\nabla}_0 \vec{E} \rangle. \quad (16)$$

It is noted here that the background does not contribute to ω_0^2 , so:

$$\vec{\nabla}_0 \vec{E}_B = 0 \quad (17)$$

and then

$$\omega_0^2 = - \frac{1}{3} \sum_{\alpha=1}^2 \left(\frac{n_\alpha q_0}{m_0} \right) \int d\vec{r} (\vec{\nabla}_0 \vec{e}_\alpha(r)) g_{0\alpha}(r) \quad (18)$$

where $g_{0\alpha}(r)$ is the pair radial distribution function for the probability of finding a ion of species α at a distance r from the impurity ion of mass m_0 and charge q_0 , n_α is the density of species α , and:

$$\vec{\nabla}_0 \cdot \vec{e}_\alpha(\vec{r}) = -\Delta U_\alpha(r) = - \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) U_\alpha(r) \quad (19)$$

$$U_\alpha(r) = \frac{q_\alpha}{r} \exp(-\bar{K}_D r) \quad (20)$$

where \bar{K}_D is the mean screening factor defined by:

$$\bar{K}_D = \left(\sum_{\alpha=1}^2 4\pi n_\alpha z_\alpha^2 \beta e^2 \right)^{1/2}. \quad (21)$$

After the substitution of these relations in (18), we obtain:

$$\omega_0^2 = -\frac{1}{3} \sum_{\alpha} \left(\frac{m_\alpha q_0}{m_0 q_\alpha} \right) \omega_{\alpha p}^2 I_{0\alpha} \quad (22)$$

where;

$$I_{0\alpha} = 1 + \int_0^\infty r \bar{K}_D^2 \exp(-\bar{K}_D r) [g_{0\alpha}(r) - 1] dr \quad (23)$$

m_α, q_α are the mass and the charge of the ion of species α .
Next, consider ω_1^2 defined by (6), (see Appendix A.2):

$$\begin{aligned} \omega_1^2 &= \left(\frac{\beta q_0^2}{3m_0 \omega_0^2} \right) \left\langle \dot{E}^2 \right\rangle \\ &= \left(\frac{q_0^2}{3m_0 \omega_0^2} \right) \left(\left\langle \left[\frac{\partial E^k}{\partial r_{0j}} \right]^2 \right\rangle \right. \\ &\quad \left. + \sum_{\alpha=1}^2 \sum_{i=1}^{N_\alpha} (m_0/m_\alpha) \left\langle \left[\frac{\partial e_\alpha^i(\vec{r}_i - \vec{r}_0)}{\partial r_{0j}} \right]^2 \right\rangle \right). \quad (24) \end{aligned}$$

To evaluate the first term on the right side of (24), we write the field at the impurity as $\vec{E} = \vec{E}' + \vec{E}_B$ and note here that the uniform background is isotropic:

$$\frac{\partial E_B^k}{\partial r_{0j}} = \frac{1}{3} \delta_{jk} \vec{\nabla}_0 \cdot \vec{E}_B \quad (25)$$

and so,

$$\begin{aligned} \left\langle \left[\frac{\partial E^k}{\partial r_{0j}} \right]^2 \right\rangle &= \\ \left\langle \left[\frac{\partial E_k'}{\partial r_{0j}} \right]^2 \right\rangle &+ \frac{1}{3} (\nabla_0 \cdot E_B)^2 + 2(\nabla_0 \cdot E_B) \langle \nabla_0 \cdot E' \rangle \quad (26) \end{aligned}$$

and then,

$$\begin{aligned} \omega_1^2 &= \left(\frac{q_0^2}{3m_0^2 \omega_0^2} \right) \sum_{\alpha=1}^2 \left(\frac{n_\alpha m_0}{\mu_\alpha} \right) \int d\vec{r} \left[\frac{\partial e_\alpha^k(\vec{r})}{\partial r_j} \right]^2 g_{0\alpha}(r) \\ &+ \frac{1}{9\omega_0^2} \left\{ \sum_{\alpha=1}^2 \left(\frac{n_\alpha q_0}{m_0} \right) \int d\vec{r} \nabla e_\alpha(r) g_{0\alpha}(r) \right\}^2 \\ &+ \left(\frac{q_0^2}{m_0^2 \omega_0^2} \right) \sum_{\alpha=1}^2 \sum_{\sigma=1}^2 n_\alpha n_\sigma \int d\vec{r} \int d\vec{r}' \left[\frac{\partial e_\alpha^k(\vec{r})}{\partial r_j} \right] \\ &\times \left[\frac{\partial e_\sigma^k(\vec{r}')}{\partial r} \right] \left\{ g_{\alpha\sigma}^{(3)}(r, r') - g_{0\alpha}(r) g_{0\sigma}(r') \right\} \quad (27) \end{aligned}$$

where $\mu_\alpha = m_0 m_\alpha / (m_0 + m_\alpha)$ is the reduced mass of pair (ion of species α -impurity ion). Via equation (18), the second term of the last formula can be simplified to give the form,

$$\begin{aligned} \omega_1^2 &= \omega_0^2 + \left(\frac{q_0^2}{3m_0^2 \omega_0^2} \right) \sum_{\alpha=1}^2 \left(\frac{n_\alpha m_0}{\mu_\alpha} \right) \int d\vec{r} \left[\frac{\partial e_{\alpha j}(r)}{\partial r_{0k}} \right]^2 g_{0\alpha}(r) \\ &+ \left(\frac{q_0^2}{3m_0^2 \omega_0^2} \right) \sum_{\alpha=1}^2 \sum_{\sigma=1}^2 n_\alpha n_\sigma \int d\vec{r} \int d\vec{r}' \left[\frac{\partial e_{\alpha j}(r)}{\partial r_k} \right] \left[\frac{\partial e_{\sigma j}(r')}{\partial r} \right] \\ &\times \left\{ g_{\alpha\sigma}^{(3)}(r, r') - g_{0\alpha}(r) g_{0\sigma}(r') \right\}. \quad (28) \end{aligned}$$

Neglecting the last term, it allows us to express ω_1^2 as:

$$\begin{aligned} \omega_1^2 &= \omega_0^2 \left(1 + \frac{q_0}{3m_0 \omega_0^4} \sum_{\alpha=1}^2 \left(\frac{n_\alpha m_0}{\mu_\alpha} \right) \right. \\ &\quad \left. \times \int d\vec{r} \left[\frac{d\vec{e}_{\alpha i}(r)}{dr_k} \right]^2 g_{0\alpha}(r) \right) \\ &= \omega_0^2 + \frac{q_0}{3m_0 \omega_0^2} \sum_{\alpha=1}^2 \left(\frac{n_\alpha m_0}{\mu_\alpha} \right) \times \int_0^\infty r^{-4} dr \exp(-2\bar{K}_D r) \\ &\quad \times \left[6 + 12\bar{K}_D r + 10(\bar{K}_D r)^2 \right. \\ &\quad \left. + 4(\bar{K}_D r)^3 + (\bar{K}_D r)^4 \right] g_{0\alpha}(r). \quad (29) \end{aligned}$$

It is understood here that the integration variable r and the screening factor \bar{K}_D^{-1} are expressed in units of the ion sphere radius a_s . The calculations proposed here are based on two approximations. The first is to neglect the last term in the expression (28). The second is the use of an empirical expression to evaluate the radial distribution function $g_{0\alpha}(r)$ [7]. The first approximation is justified and acceptable because the neglected term deals with a three body interaction for which the corresponding third function is small with respect to the pair function ($g^{(3)} \ll g^{(2)}$). The second approximation is well justified for strong coupling and it is simplest to work with the Coulomb radial function $g_{0\alpha}(r)$ given by [7] instead of the screened radial function for which we do not have an analytical expression.

Finally, thanks to the ‘‘disconnected approximation’’ for the collisional operator [11], we obtain the self-coefficient diffusion D as:

$$\begin{aligned} D^{-1} &= \\ \frac{1}{6\pi m_i} \sum_{\alpha, \beta} \int_0^\infty k^4 dk \tilde{V}_{0i\alpha}(k) \tilde{C}_{0\beta}(k) \int_{-\infty}^{+\infty} d\omega S_{\alpha\beta}(k, \omega) S_0^s(k, \omega) \quad (30) \end{aligned}$$

where $S_{\alpha\beta}(k, \omega)$ is the dynamic structure factor for density fluctuations in species α and β , $S_0^s(k, \omega)$ is the self-structure factor for the impurity ion that is taken as:

$$S_0^s(k, \omega) = (1/k)(\pi\beta m_0/2)^{1/2} \exp(-m\beta\omega^2/(2k^2)). \quad (31)$$

$$\begin{aligned}
S_{11} &= \frac{n_1 \left[1 + n_1 \widehat{h}_{11}(k) \right] I_1 \left[1 - n_2 \widehat{c}_{22}(k)(1 - ZI_2) \right] + n_2 n_1^2 \widehat{c}_{12}(k) \widehat{h}_{12}(k)(1 - ZI_1) I_2}{\left[1 - n_1 \widehat{c}_{11}(k)(1 - ZI_1) \right] \left[1 - n_2 \widehat{c}_{22}(k)(1 - ZI_2) \right] - n_1 n_2 \widehat{c}_{12}^2(k)(1 - ZI_2)(1 - ZI_1)} \\
S_{22} &= \frac{n_2 \left[1 + n_2 \widehat{h}_{22}(k) \right] I_2 \left[1 - n_1 \widehat{c}_{11}(k)(1 - ZI_1) \right] + n_1 n_2^2 \widehat{c}_{12}(k) \widehat{h}_{12}(k)(1 - ZI_2) I_1}{\left[1 - n_1 \widehat{c}_{11}(k)(1 - ZI_1) \right] \left[1 - n_2 \widehat{c}_{22}(k)(1 - ZI_2) \right] - n_1 n_2 \widehat{c}_{12}^2(k)(1 - ZI_2)(1 - ZI_1)} \\
S_{21} &= \frac{n_1 n_2 \widehat{h}_{12}(k) I_2 \left[1 - n_1 \widehat{c}_{11}(k)(1 - ZI_1) \right] + n_2 n_1 \widehat{c}_{12}(k)(1 - ZI_2) I_1 \left[1 + n_1 \widehat{h}_{11}(k) \right]}{\left[1 - n_1 \widehat{c}_{11}(k)(1 - ZI_1) \right] \left[1 - n_2 \widehat{c}_{22}(k)(1 - ZI_2) \right] - n_1 n_2 \widehat{c}_{12}^2(k)(1 - ZI_2)(1 - ZI_1)} \\
S_{12} &= \frac{n_1 n_2 \widehat{h}_{12}(k) I_1 \left[1 - n_2 \widehat{c}_{22}(k)(1 - ZI_2) \right] + n_2 n_1 \widehat{c}_{12}(k)(1 - ZI_1) I_2 \left[1 + n_2 \widehat{h}_{22}(k) \right]}{\left[1 - n_1 \widehat{c}_{11}(k)(1 - ZI_1) \right] \left[1 - n_2 \widehat{c}_{22}(k)(1 - ZI_2) \right] - n_1 n_2 \widehat{c}_{12}^2(k)(1 - ZI_2)(1 - ZI_1)}. \tag{37}
\end{aligned}$$

$\widetilde{V}_{0\alpha}(k)$ is the Fourier transform of the pair potential interaction of the impurity with an ion of species α , and $\widetilde{C}_{0\alpha}(k)$ is the corresponding Fourier transform of the direct correlation function for the interaction with species α ,

$$\widetilde{C}_{0\alpha}(k) = -\beta \widetilde{V}_{0\alpha}(k). \tag{32}$$

Now we need the expression of the dynamic structure factor $S_{\alpha\beta}(k, \omega)$ of the density fluctuation in species α and β . These factors can be derived from kinetic theory as follows.

All the transport phenomena can be obtained from kinetic equations of transport [10,11]:

$$\begin{aligned}
\left(z + i \frac{\vec{k} \cdot \vec{p}}{m_\alpha} \right) S_{\alpha,\beta}(\vec{k}, z, \vec{p}, \vec{p}') &= \\
- i \sum_{\sigma=1}^2 \int d\vec{p}'' \Phi_{\alpha,\sigma}(\vec{k}, z, \vec{p}, \vec{p}'') S_{\sigma,\beta}(\vec{k}, z, \vec{p}', \vec{p}'') & \\
+ n_\alpha \phi_\alpha(\vec{p}) \left[\delta_{\alpha,\beta} \delta(\vec{p} - \vec{p}') + n_\beta h_{\alpha\beta}(\vec{k}) \phi_\beta(\vec{p}') \right] & \tag{33}
\end{aligned}$$

where $\phi_\alpha(p)$ is the Maxwell-Boltzmann distribution for species α and $h_{\alpha\beta}(k)$ is the Orstein-Zernike pair function defined by:

$$h_{\alpha\beta}(k) = \int d\vec{r} \exp(i\vec{k} \cdot \vec{r}) (g_{\alpha\beta}(r) - 1) \tag{34}$$

and the kernel $\Phi_{\alpha,\sigma}(k, z, p, p'')$ is the collision operator defined by:

$$\Phi_{\alpha,\sigma}(k, z, p, p'') = -n_\alpha \frac{kp}{m_\alpha} \phi_\alpha(p) C_{\alpha\sigma}(k) + M_{\alpha\sigma}(k, z, p, p''). \tag{35}$$

In our model we shall keep only the first term on the righthand side of the last equation. After inserting the expression for $\Phi_{\alpha,\sigma}(k, z, p, p'')$ in (33) and integrating out over the momentum p and p' , we obtain a closed system of four autonomous algebraic equations for $S_{\alpha\beta}$:

$$\begin{aligned}
n S_{\alpha\beta}(k, z) &= \\
i \int dp \frac{n_\alpha (kp/m_\alpha)}{z + i(kp/m_\alpha)} \phi_\alpha(p) \sum_{\sigma=1}^2 n S_{\sigma\beta}(k, z) C_{\alpha\sigma}(k) & \\
+ (in_\alpha \delta_{\alpha\beta} + n_\alpha n_\beta h_{\alpha\beta}(k)) \int dp \frac{\phi_\alpha(p)}{z + i(kp/m_\alpha)} & \tag{36}
\end{aligned}$$

for which the solutions are:

See equation (37) above.

In principle, these results enable us to calculate the diffusion coefficient D . By substituting (31), (34) and (37) in (39) we can also calculate the parameter λ :

$$\begin{aligned}
\lambda &= \frac{1}{m_0 \beta} (\omega_1^2 / \omega_0^2 - 1) D^{-1} \\
&= \left(\frac{\omega_1^2 / \omega_0^2 - 1}{6\pi\beta m_0^2} \right) \sum_{\alpha,\beta} \int_0^\infty k^4 dk \widetilde{V}_{0\alpha}(k) \widetilde{C}_{i\beta}(k) \\
&\quad \times \int_{-\infty}^{+\infty} d\omega S_{\alpha\beta}(k, \omega) S_0^s(k, \omega). \tag{38}
\end{aligned}$$

Once the three parameters ω_0 , ω_1 and λ are obtained we are able to find the cubic equation solutions of (14) and discuss their relationships with the dynamic properties.

4 Discussion and results

We have presented a model for the auto-correlation function $C(t)$ of the electric field at the impurity and $D(t)$ of the velocity of the impurity in TICP. This model is based on the exact master equation (5) and the second derivative equation (4). The self-diffusion coefficient is treated by the velocity autocorrelation function and the Green-Kubo relation (8). However, as seen in Figures 1 and 2, the function $D(t)$ is slowly decaying and its time integral requires a long simulation time.

In our model, we have started to compute the diffusion coefficient in two different ways. The first is related to the static and dynamical structure factors via formula (30). The second is related to the Molecular Dynamics Simulation (MDS). The result is found to be in good agreement for different coupling parameters and different concentrations see Tables 1, and 2.

At the second stage, we compute theoretically the autocorrelation functions through solving the algebraic cubic equation (14). We find in general three solutions. In the case of a strong coupling parameter Γ , two of these solutions (modes) are complex (z, z^*) and the microfield

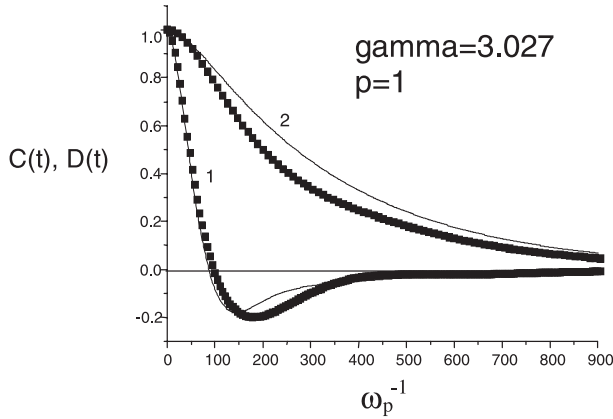


Fig. 1. Autocorrelation microfield function $C(t)$ (1) and autocorrelation velocity function $D(t)$ (2) of a pure Ar(17+) with $\Gamma = 3.027$. (.....) the simulation and (—) our model.

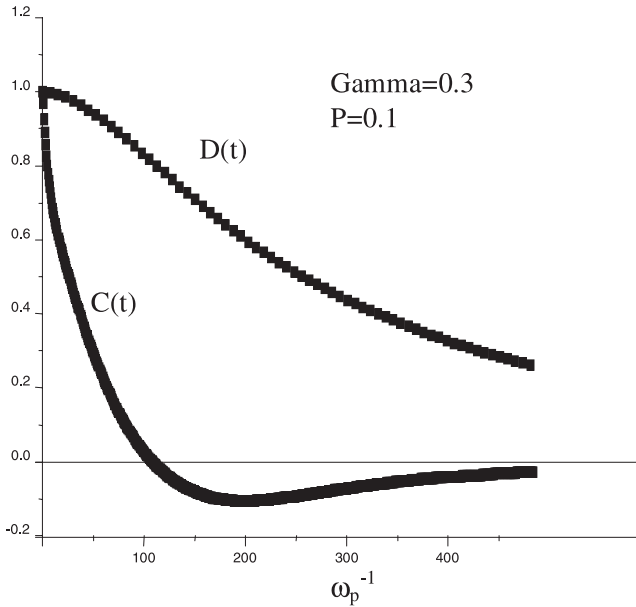


Fig. 2. Autocorrelation microfield function $C(t)$ and Autocorrelation velocity function $D(t)$ of a Ar(17+) at concentration $p = 0.1$ in He(+), with $\Gamma = 0.3$. (.....) the simulation and (—) our model.

autocorrelation function $C(t)$ exhibits an important time oscillation with a frequency equal to imaginary part of the complex solution. While the real part expresses the time decay (damping) of $C(t)$ or one can equally say, the time decay of the memory effect due to the interaction of the impurity with the medium. In the weak coupling parameter Γ , the three solutions are real, and the oscillations of $C(t)$ become very slow and disappear when the coupling Γ goes to zero and the damped regime takes place.

In Figures 1, 2 and 3, we have presented the autocorrelation functions both for the electric field at the impurity and the velocity of the impurity in TICP. We show a good agreement between those obtained by MDS developed in our laboratory PIIM and our theoretical model. The cal-

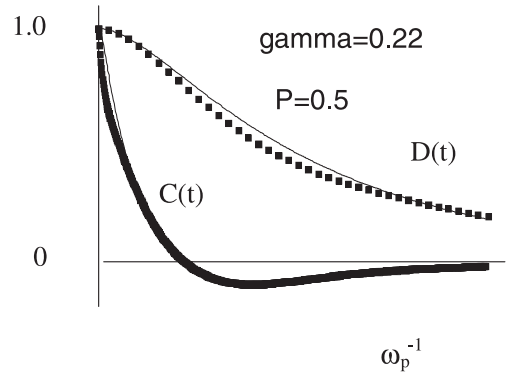


Fig. 3. Autocorrelation microfield function $C(t)$ and Autocorrelation velocity function $D(t)$ of a Ar(17+) at concentration $p = 0.5$ in He(+), with $\Gamma = 0.22$. (.....) the simulation and (—) our model.

Table 2. Diffusion coefficient of He⁺² in (50%He⁺², 50%H⁺¹) with different coupling.

Γ	$D^*(\text{model})$	D_{MD}
0.02	231.827	223.75
0.04	78.52	71.08
0.2	7.58	6.20
1.00	0.91	0.75

culaton and the comparison have also been made for different concentrations of the mixture (Ar17+/He+) and different coupling parameter Γ (gamma). Nevertheless, we mention that there is a bit of a difference between the theoretical model and the MDS in the case of weak coupling. This may be due to an inadequacy in the theoretical model regarding, as we know, the use of $g_{0\alpha}(r)$ which is suitable only for strong coupling.

In conclusion, we have presented a model which provides an exact autocorrelation function both for the electric field at the impurity and the velocity of the impurity. The comparison of the Dynamic Molecular Simulation (DMS) results with those obtained in the model shows a good agreement. The comparison was made and extended to many values of the physical parameters like the coupling gamma, concentration of the impurity $p = n_2/(n_1 + n_2)$ whereas the electronic density n was fixed. The agreement with the DMS should provide a very powerful tool to investigate many dynamic properties and transport phenomena in ionized media such as a plasma and electrolytic solutions.

Appendix A

A.1 Establishment of the master equation for $D(t)$

The velocity autocorrelation function obeys a general equation (5). This equation is derived using the Zwanzig projection operator. One is interested in a dynamic variable (position, velocity, field...) $y_\alpha(t)$ which obeys the

Liouville equation:

$$y_\alpha(t) = \exp(Lt)y_\alpha(0), Ly_\alpha = \{y_\alpha, H\}. \quad (39)$$

The time derivative of (39) is:

$$\frac{dy_\alpha(t)}{dt} = Ly_\alpha(t). \quad (40)$$

A projection operator P is defined as [6]

$$Px = y_\alpha g_{\alpha\beta}^{-1} \langle y_\beta x \rangle, \text{ with } g_{\alpha\beta} = \langle y_\alpha y_\beta \rangle. \quad (41)$$

Applying this projection operator to the equation (40), we find:

$$P\dot{y}_\alpha(t) = PL[Py_\alpha(t) + (1-P)y_\alpha(t)]. \quad (42)$$

Putting: $Z_\alpha(t) = Py_\alpha(t)$ and $W_\alpha(t) = (1-P)y_\alpha(t)$, then:

$$W_\alpha(t) = \exp(QLQt)W_\alpha(0) + \int_0^t \exp(QLQ(t-\tau))LPZ_\alpha(\tau)d\tau. \quad (43)$$

Since $Q = 1 - P$ is also a projection operator, one can write

$$\dot{Z}_\alpha(t) = PLZ_\alpha(t) + PL \int_0^t \exp(QLQ(t-\tau))LPZ_\alpha(\tau)d\tau. \quad (44)$$

As: $PZ_\alpha(\tau) = P^2y_\alpha(\tau) = Py_\alpha(\tau)$, then:

$$P\dot{y}_\alpha(t) = PLPy_\alpha(t) + PL \int_0^t \exp(QLQ(t-\tau))LPy_\alpha(\tau)d\tau \quad (45)$$

which is translated by

$$P \left\{ \dot{y}_\alpha(t) - LPy_\alpha(t) - L \int_0^t \exp(QLQ(t-\tau))LPy_\alpha(\tau)d\tau \right\} = 0 \quad (46)$$

or:

$$\dot{y}_\alpha(t) = LPy_\alpha(t) + L \int_0^t \exp(QLQ(t-\tau))LPy_\alpha(\tau)d\tau. \quad (47)$$

Let's multiply the equation (47) on the left by y_β and carry out the statistical Gibbs average:

$$\langle y_\beta \dot{y}_\alpha(t) \rangle = \langle y_\beta LPy_\alpha(t) \rangle + \left\langle y_\beta L \int_0^t \exp(QLQ(t-\tau))LPy_\alpha(\tau)d\tau \right\rangle. \quad (48)$$

If we put:

$$K_{\beta\alpha}(t) = \langle y_\beta y_\alpha(t) \rangle \quad (49)$$

and apply the definition (41) for the computation of the derivative of $K_{\beta\alpha}(t)$, we obtain a master equation:

$$\frac{dK_{\beta\alpha}(t)}{dt} = \Omega_{\beta\sigma} K_{\sigma\alpha}(t) + \int_0^t M_{\beta\sigma}(t-\tau)K_{\sigma\alpha}(\tau)d\tau \quad (50)$$

where:

$$\begin{aligned} \Omega_{\beta\sigma} &= \langle y_\beta Ly_\gamma \rangle g_{\gamma\sigma}^{-1} \text{ and } M_{\beta\sigma}(u) \\ &= \langle y_\beta L \exp(QLQ(u))Ly_\gamma \rangle g_{\gamma\sigma}^{-1}. \end{aligned} \quad (51)$$

When choosing the matrix $[g]$ as [6]:

$$g_{\alpha\beta} = \delta_{\alpha\beta} g_{\alpha\alpha}, \text{ where } g_{11} = \langle V_0^2 \rangle \text{ and } g_{22} = \langle E^2 \rangle \quad (52)$$

one can show the following results:

$$\Omega_{11} = \Omega_{22} = 0, \quad \Omega_{12} = -\frac{Z_0 e}{m_0}, \quad \Omega_{21} = \frac{Z_0 e \langle E^2 \rangle}{m_0 \langle V_0^2 \rangle}$$

and

$$\begin{aligned} M_{11}(u) &= M_{22}(u) = M_{21}(u) = 0, \\ M_{22}(0) &= -(\omega_1^2 - \omega_0^2). \end{aligned}$$

Putting $\beta = 2$ in the equation (50) and using the results in (51), we obtain:

$$\frac{dK_{2\alpha}(t)}{dt} = \Omega_{21} K_{1\alpha}(t) + \int_0^t M_{22}(t-\tau)K_{2\alpha}(\tau)d\tau \quad (53)$$

and using:

$$\begin{aligned} \frac{dK_{1\alpha}(t)}{dt} &= \frac{d}{dt} \langle y_1 y_\alpha(t) \rangle = \frac{d}{dt} \langle y_1(-t) y_\alpha(0) \rangle \\ &= -\frac{Z_0 e}{m_0} \langle y_2 y_\alpha(t) \rangle = -\frac{Z_0 e}{m_0} K_{2\alpha}(t) \end{aligned} \quad (54)$$

and so after substituting the equation (54) in (53) and putting $\alpha = 1$, we find equation (5)

$$\left\{ \frac{d^2}{dt^2} + \frac{(Z_0 e)^2 \langle E^2 \rangle}{m_0^2 \langle V^2 \rangle} \right\} D(t) - \int_0^t M_{22}(t-\tau) \frac{dD(\tau)}{dt} d\tau = 0. \quad (55)$$

A.2 Evaluation of ω_1^2

The parameter ω_1^2 is defined by the equation (6):

$$\begin{aligned} \omega_1^2 &= \left(\frac{\beta q_0}{3m_0 \omega_0^2} \right) \left\langle \dot{E}^2(0) \right\rangle \\ &= \left(\frac{\beta q_0^2}{3m_0 \omega_0^2} \right) \left\langle \frac{dE_k(0)}{dt} \frac{dE_k(0)}{dt} \right\rangle \end{aligned} \quad (56)$$

where the repeated indices stand for the sum on k .

$$\frac{dE_k(0)}{dt} = \sum_{\alpha} \sum_{i=1}^{N_{\alpha}} \frac{\partial e_{\alpha}^k(\vec{r}_i - \vec{r}_0)}{\partial r_{0j}} \frac{d(\vec{r}_i - \vec{r}_0)}{dt} + \frac{\partial E^k(\vec{r}_0)}{\partial r_{0j}} \frac{d\vec{r}_0}{dt}$$

or again after some arrangements:

$$\frac{dE_k(0)}{dt} = \sum_{\alpha} \sum_{i=1}^{N_{\alpha}} \vec{V}_i^j \frac{de_{\alpha}^k(\vec{r}_i - \vec{r}_0)}{d\vec{r}_{0j}} + \vec{V}_0^j \frac{dE^k(\vec{r}_0)}{dr_{0j}}$$

which finally gives the expression:

$$\omega_1^2 = \sum_{\alpha} \sum_{i=1}^{N_{\alpha}} \frac{m_{\alpha}}{m_0} \left\langle \left(\frac{\partial e_{\alpha}^k(\vec{r}_i - \vec{r}_0)}{\partial \vec{r}_{0j}} \right)^2 \right\rangle + \frac{q_0^2}{3m_0^2\omega_0^2} \left\langle \left(\frac{\partial E^k(\vec{r}_0)}{\partial \vec{r}_{0j}} \right)^2 \right\rangle \quad (57)$$

we notice that the second term of the second member can be written otherwise:

$$\begin{aligned} \frac{\partial E^k(\vec{r}_0)}{\partial r_{0j}} &= \sum_{\alpha} \sum_{i=1}^{N_{\alpha}} \frac{\partial e_{\alpha}^k(\vec{r}_i - \vec{r}_0)}{\partial r_{0j}} + \frac{\partial E_B^k(\vec{r}_0)}{\partial r_{01}} \\ &= \frac{\partial e_{\alpha}^k(\vec{r}_0)}{\partial r_{01}} + \frac{1}{3} \delta_{k1} \nabla_0 E_B^k(\vec{r}_0) \end{aligned} \quad (58)$$

with

$$\vec{\nabla}_0 \vec{E}_B(\vec{r}_0) = 0, \quad (59)$$

then

$$\omega_1^2 = \sum_{\alpha} \sum_{i=1}^{N_{\alpha}} \frac{m_{\alpha}}{m_0} \left\langle \left(\frac{\partial e_{\alpha}^k(\vec{r}_i - \vec{r}_0)}{\partial \vec{r}_{0j}} \right)^2 \right\rangle + \frac{q_0^2}{3m_0^2\omega_0^2} \sum_{\alpha} \sum_{i=1}^{N_{\alpha}} \left\langle \left(\frac{\partial e_{\alpha}^k(\vec{r}_i - \vec{r}_0)}{\partial \vec{r}_{0j}} \right)^2 \right\rangle. \quad (60)$$

The last expression involves N identical terms in the sum, if we compute the average for one term:

$$\begin{aligned} \left\langle \left(\frac{\partial e_{\alpha}^k(\vec{r}_i - \vec{r}_0)}{\partial \vec{r}_{0j}} \right)^2 \right\rangle &= \\ \int d\vec{r}_0 d\vec{r}_1 \dots d\vec{r}_N \rho_{eq} \left(\frac{\partial e_{\alpha}^k(\vec{r}_i - \vec{r}_0)}{\partial \vec{r}_{0j}} \right)^2 & \quad (61) \end{aligned}$$

and we change the integration variables:

$$\frac{\vec{r}_i - \vec{r}_0}{2} = \vec{r} \quad \text{and} \quad \frac{\vec{r}_i + \vec{r}_0}{2} = \vec{R} \quad (62)$$

we find:

$$\begin{aligned} \omega_1^2 &= \frac{1}{9\omega_0^2} \left\{ \sum_{\alpha} \left(\frac{n_{\alpha} q_0}{m_0} \right) \int d\vec{r} \vec{\nabla}_0 \cdot \vec{e}_{\alpha}(\vec{r}) g_{0\alpha}(r) \right\}^2 \\ &+ \frac{q_0^2}{3m_0^2\omega_0^2} \sum_{\alpha} \left(\frac{n_{\alpha} m_0}{\mu_{0\alpha}} \right) \sum_{i=1}^{N_{\alpha}} \int d\vec{r} \left(\frac{\partial e_{\alpha}^k(\vec{r})}{\partial r_j} \right)^2 g_{0\alpha}(r) \\ &+ \left(\frac{q_0}{3m\omega_0} \right)^2 \sum_{\alpha} \sum_{\sigma} n_{\alpha} n_{\sigma} \int d\vec{r} d\vec{r}' \left(\frac{\partial e_{\alpha}^k(\vec{r})}{\partial r_j} \right) \\ &\times \left(\frac{\partial e_{\sigma}^k(\vec{r}')}{\partial r_j} \right) \left(g_{\alpha\sigma}^{(3)}(\vec{r}, \vec{r}') + g_{\alpha}(r) g_{\sigma}(r') \right) \end{aligned}$$

here $\mu_{0\alpha}$ is the reduced mass and $g_{0\alpha}(r)$ is the distribution function of the pair (impurity ion-ion of species α) and finally the parameter ω_1^2 is given by:

$$\begin{aligned} \omega_1^2 &= \omega_0^2 + \frac{q_0^2}{3m_0^2\omega_0^2} \\ &\times \sum_{\alpha} \left(\frac{n_{\alpha} m_0}{\mu_{0\alpha}} \right) \sum_{i=1}^{N_{\alpha}} \int d\vec{r} \left(\frac{\partial e_{\alpha}^k(\vec{r})}{\partial r_j} \right)^2 g_{0\alpha}(r) \\ &+ \left(\frac{q_0}{3m\omega_0} \right)^2 \sum_{\alpha} \sum_{\sigma} n_{\alpha} n_{\sigma} \int d\vec{r} d\vec{r}' \left(\frac{\partial e_{\alpha}^k(\vec{r})}{\partial r_j} \right) \\ &\times \left(\frac{\partial e_{\sigma}^k(\vec{r}')}{\partial r_j} \right) \left(g_{\alpha\sigma}^{(3)}(\vec{r}, \vec{r}') + g_{\alpha}(r) g_{\sigma}(r') \right). \quad (63) \end{aligned}$$

Neglecting the third term in the last formula and performing the divergence calculus in the second term (using the screened potential), we obtain:

$$\begin{aligned} \omega_1^2 &= \omega_0^2 + \frac{q_0^2}{3m_0^2\omega_0^2} \\ &\times \sum_{\alpha} \left(\frac{n_{\alpha} m_0}{\mu_{0\alpha}} \right) \sum_{i=1}^{N_{\alpha}} \int d\vec{r} \left(\frac{\partial e_{\alpha}^k(\vec{r})}{\partial r_j} \right)^2 g_{0\alpha}(r). \end{aligned}$$

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