Slow and fast micro-field components in warm and dense hydrogen plasmas

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Abstract

The aim of this work is the investigation of the statistical properties of local electric fields in an ion-electron two component plasmas for coupled conditions. The stochastic fields at a charged or at a neutral point in plasmas involve both slow and fast fluctuation characteristics. The statistical study of these local fields based on a direct time average is done for the first time. For warm and dense plasma conditions, typically \( N_e \approx 10^{18}\text{cm}^{-3} \), \( T_e \approx 1\text{eV} \), well controlled molecular dynamics (MD) simulations of neutral hydrogen, protons and electrons have been carried out. Relying on these \textit{ab initio} MD calculations this work focuses on an analysis of the concepts of statistically independent slow and fast local field components, based on the consideration of a time averaged electric field. Large differences are found between the results of these MD simulations and corresponding standard results based on static screened fields. The effects discussed are of importance for physical phenomena connected with stochastic electric field fluctuations, e.g., for spectral line broadening in dense plasmas.

PACS numbers: 52.65.-y, 52.25.Ya
The study of the local stochastic electric fields at neutral or charged points in an homogeneous infinite plasma is of interest for several domains. For instance they can be used as external perturbations within semiclassical models designed to synthesize line spectra for diagnostic purposes \[1,2,3,4\]. A more general interest comes with the study of non linear dynamics of charges undergoing the corresponding forces. This work addresses the simpler problem of an hydrogen plasma and the analysis of the local field at neutral points. An equivalent study of the local field measured at charged points is straightforward.

The mass ratio between electrons and protons results in fields involving both fast and slow fluctuations characteristics. In order to analyze the statistical properties of these fields, a couple of components, a slow-fluctuation component (S) and a fast-fluctuation component (F) is introduced,

\[
E(t) = E_e(t) + E_i(t) = E_{\text{slow}}(t) + E_{\text{fast}}(t),
\]

where \(E_e\) and \(E_i\) are the fields due to the electrons and ions, respectively, at an arbitrary neutral point. Our objective is to suggest a natural definition of the slow and fast components and then determine their statistical properties, subject to the constraints 1) their sum must be the total field, 2) they must be statistically independent. Years ago, S and F components have been defined in well known articles \[5,6,7,8\] (BMHH) and this will be referred to as the standard model. The present work exploits plasma molecular dynamics simulations (MD) with a more precise definition that will be referenced as ab initio method.

The long history of plasma spectroscopy has provided indirect interpretations of the static and dynamic properties of the local field through their action on the relaxation of a line emitted by the plasma \[9,10\]. However, the plasma and atomic state averages required do not allow detailed information relevant to the splitting of the field into S and F components. In contrast, MD simulation provides a means for direct access to such information. The results presented here are based on the analysis of the stochastic fluctuations of sums and differences of the ionic and electronic local fields, \(E_i(t), E_e(t)\) and the time averaged electron field

\[
\overline{E_e(t)}_{\Delta t} = \frac{1}{\Delta t} \int_{-\Delta t/2}^{\Delta t/2} E_e(t - t') dt'.
\]

The mean electronic field, \(\overline{E_e(t)}_{\Delta t}\), calculated on variable periods of time, \(\Delta t\), can be considered also as a simple measurement device, with variable response time, averaging out on the fast fluctuation of the total field due to the electrons. The reason for introducing this
average field is clearly to filter the total field and identify the S and F components Accordingly, the slow component is defined here as the slowly varying ion field plus the residual slowly varying mean electron field

\[ E_{S,\Delta t}(t) = E_i(t) + \overline{E_e(t)}\Delta t. \] (3)

The fast component is the remainder \( E_{F,\Delta t}(t) = E(t) - E_{S,\Delta t}(t) = E_e(t) - \overline{E_e(t)}\Delta t. \) The justification for this decomposition is provided by the simulation results below.

MD simulation of a partially ionized hydrogen plasma gives the local ion, electron and total fields at neutral hydrogen atoms. The density and temperature conditions are chosen to explore rather coupled conditions: \( N_e \approx 10^{18} \text{ cm}^{-3} \) and \( T_e \approx 1 \text{ eV} \). Simulations of infinite systems are achieved with periodic boundary conditions. Coulomb interactions are shielded at a distance \( \lambda \approx s/2 \), of the order of the cubic MD cell size \( s \), large enough to allow natural screening, e.g., Debye screening, and to not affect appreciably any of the properties investigated below. The ion-ion and electron-electron repulsive interactions are given by a shielded Coulomb potential \( V_{12}(r) = e^2 e^{-r/\lambda}/r \). Attractive electron-ion Coulomb interactions are regularized as follows: \( V_{ie}(r) = -e^2 (1 - e^{-r/\delta}) e^{-r/\lambda}/r \), the short range regularization parameter \( \delta \) is such that the potential energy of an electron sited on top of a proton is equal to the ionization energy of a hydrogen atom [11]. Regularization allowing to implement a Coulomb attractive potential in MD simulations has proven useful [12, 13].

Parameters of interest are the electron-electron or ion-ion average distance, \( r_0 = (3/4\pi N_e)^{1/3} \), defined in terms of the electron density \( N_e \), the mean electric field modulus \( E_0 = e/r_0^2 \), the electron thermal velocity \( v_0 = (k_B T_e/m_e)^{1/2} \), the electron and proton coupling constant \( \Gamma = e^2/r_0 k_B T_e \) and the Debye length \( \lambda_D = (k_B T_e/4\pi N_e e^2)^{1/2} \).

Two plasma conditions have been considered, which correspond to \( \alpha = 0.8 \) and \( \alpha = 0.4 \), where \( \alpha = r_0/\lambda_D \) is the parameter introduced in BMHH. Both cases, with a same temperature of 1eV and coupling parameters \( \Gamma \approx 0.2 \) and \( \Gamma \approx 0.06 \), correspond to realistic experimental plasma conditions. The number of electrons is \( \approx 1000 \) with box sizes \( s > 3\lambda_D \). The same time-step \( t = 1.5 \times 10^{-17} \text{s} \) has been used for ions and electrons. This implies that, for \( \alpha = 0.8 \), 11600 time-steps are required for a proton to move across \( r_0 \) (270 for an electron). These parameters give rise to intensive simulations that typically run over a few \( 10^7 \) time-steps. Times for ions and electrons to cross the mean distance provide the ionic and electronic characteristic times \( \tau_i \approx 10^{-12} \text{s} \) and \( \tau_e \approx 10^{-14} \text{s} \) of fluctuations of local fields,
since the field correlation is lost, in average, once particles have moved across the mean distance. A careful preparation of positions and velocities of charges inside the simulation cell guarantees a good stationarity of the total energy all along a simulation. Typically, the relative variation of the total energy over a simulation is smaller than 1%. The analysis of the time averaged electron field introduces new complications beyond those of current two component MD simulations and these have been addressed with care.

In Fig. 1 three field correlation functions have been plotted on the same graph in units of $\tau_e$, for the case $\alpha = 0.8$: $\langle E_e(0)E_e(t) \rangle$, (circles), $\langle E_i(0)E_e(t) \rangle$, (black circles) and $\langle E_{F,\Delta t}(0)E_{F,\Delta t}(t) \rangle$, (crosses) for $\Delta t = 0.4\tau_e$. The symbol $\langle \rangle$ denotes a statistical average on a relevant set of independent field histories built, according to the present simulation method, both at different times and for different neutral points. Clearly, in the framework of two component plasmas, the electron field appears inappropriate to represent the F component as the corresponding field correlation function manifestly shows a slow de-correlation due to electron-ion coupling mechanisms [10, 13], implying a statistical dependency between ion and electron fields. In contrast, the correlation of $E_{F,\Delta t}(t)$ with $\Delta t = 0.4\tau_e$ is lost over a time $< \tau_e$ (estimated only roughly because of the noise). The definitions for the S and F components depend on $\Delta t$. It will be understood hereafter that the fast and slow characteristics of fields can get a more precise meaning by comparison to an additional time $\tau$ connected to some physical process, e.g., the relaxation of a plasma density fluctuation or the relaxation of an atomic radiation due to atom emitters imbedded in the plasma. The
present S and F component definitions make sense mainly for processes with \( \tau_e < \tau < \tau_i \), i.e., for components with fluctuation times roughly connected to those of ions and electrons. For instance, cases such that \( \tau_i \ll \tau, \tau \ll \tau_e \) or \( \tau_i = \infty \) are not really considered in this work.

The attractive interaction between ions and electrons gives rise to an average response of the electrons to a ionic field polarizing locally the plasma. This average response corresponds to a natural anti-correlation mechanism i.e. \( \langle \mathbf{E}_i(0), \mathbf{E}_e(t) \rangle < 0 \) plotted in Fig.1 and also clearly shown in [10]. This gives rise to the well-known model based on screening of ion-ion interactions by the fast moving electrons. In the standard model the slow component is taken to be a screened ion field, with a screening length due to the electrons. A primary observation here is that this definition of the slow component does not agree with that of Eq.(3). More precisely, the static screening effect is not equivalent to the time average of the electronic motion. A further approximation in applications of the standard model is to replace the corresponding fast component by that due to the electrons alone. The results below provide significant motivation for reconsideration of those applications, particularly in light of the early identification of screening with time averages.

In order to clarify the following comparisons it is useful to recall a few preliminary notions. The Holtsmark function [14] gives the field distribution function (FDF) inside an infinite space filled with a uniform random distribution of point charges \( Z = \pm 1 \) at a density \( N \). For instance the Holtsmark curve is the FDF inside an infinite system of noninteracting electrons at a density \( N_e = N \) while the total ion plus electron FDF, still for noninteracting charges, is given by the Holtsmark distribution for the density \( 2N \). It is well known that when the interaction between charges are switched on the average field modulus decreases. This effect is accentuated by increasing plasma coupling conditions.

In the two component plasma investigated here, with all the interactions accounted for, the electronic and the ionic FDFs are also remarkable. Due to the symmetry of charges they are the same. In addition, when \( \Delta t \) increases, the FDFs of both \( \mathbf{E}_{F,\Delta t}(t) \) and \( \mathbf{E}_{S,\Delta t}(t) \) tend towards the common electronic and ionic FDF (IEFDF) as, due to ergodicity \( \lim_{\Delta t \to \infty} \mathbf{E}_e(t)_{\Delta t} = \langle \mathbf{E}_e(t) \rangle = 0 \). The statistical independency of the S and F components is effective as demonstrated in Fig.1.

Figure 2 is a typical illustration of the central problem of this work. Three FDFs of the S component (solid lines), i.e., of the field \( \mathbf{E}_{S,\Delta t}(t) = \mathbf{E}_i(t) + \mathbf{E}_e(t)_{\Delta t} \) have been obtained with
FIG. 2: S component field distribution functions at neutral emitters, $\alpha = 0.8$

FIG. 3: F component field distribution functions for $\alpha = 0.8$, $\Delta t$ increases from the left to the right; dash: electron FDF

various integration times $\Delta t$. The S component shows a small dependence on $\Delta t$ around $\tau_e$, suggesting that the smallest time interval contains already most of the contribution of electrons to the S component. The strong field wings are located in between the two Holtsmark curves (circles) as the slow fields result from interacting charged particles at a density $2N_e$. The limit of the S component for increasing $\Delta t$ is the ion field distribution function (dash). As commented above, this ionic FDF resulting from interacting ions at a density $N_e$ is shifted towards smaller field modulus with respect to the Holtsmark curve (black circles). Finally, for comparison, the field distribution function labelled "Hooper" (dotted curve) which represent the standard model, obtained with ionic field at emitters
screened at the Debye length, has been plotted. The large difference observed with the present model gauges the consequences of the definition that funds the standard model.

In the same way, the F field distribution function can be extracted from MD simulations. In Fig. 3 when $\Delta t$ increases the FDF is shifted from small fields to the electron FDF, i.e., the limit obtained when $\Delta t$ increases. According to the standard model, the electron FDF gives the F component.

An equivalent behavior is found for the case $\alpha = 0.4$. Figure 4 shows the S field distribution function obtained with a time-average length $\Delta t = \tau_e$ together with the Holtsmark distributions and the ion field distribution. As in the $\alpha = 0.8$ case the strong field wing of the S field distribution function lays in between the two Holtsmark curves. These calculations for two distinct coupling conditions show that as expected, the Hooper S component, the ionic FDF and the Holtsmark FDF get closer as $\Gamma$ decreases.

Coming back to the scope of this work a few points should be kept in mind. This preliminary work exploits intensive relevant MD sampling of stochastic local-fields at neutral points in an hydrogen plasma for two distinct density-temperature conditions. Studies for other conditions would be useful. However, our objective here, i.e., the study of the statistical properties of these sampled field in order to be able to discuss existing models, has been reached. Due to the masses involved, local fields undergo an intricate superposition of fast and slow fluctuations. This suggests a rational method based on the mean electron field for the splitting of the total field into a couple of statistically independent S and F components whose statistical properties are investigated separately. The procedure leading to the S/F
splitting is straightforward as it basically averages out the fast fluctuation on variable periods of time. In contrast, the standard BMHH procedure uses an S component rendered with an average ionic potential involving a screening term to account for ions dressed by electrons. The S component standard model therefore is a purely ionic field, while that for the ab initio method entangles both ions and those of the electrons contributing to slow fields. Clearly, the MD ab initio approach is able to show the anti-correlation mechanisms understood in the standard model by the screening term implemented in the average ionic potential but does not lead to the standard model itself, even as a limit process. The consequence is that both approaches result in distinct models for the FDFs.

Simple comparisons can be performed using the common IEFDF plotted in Figs. 2 and 3 with dash lines. This curve i.e., the limit reached by $E_{S,\Delta t}(t)$ and $E_{F,\Delta t}(t)$ when $\Delta t$ increases, represents a S and a F component which are not statistically independent as inferred from Fig. [1]. For any $\Delta t > 0$, the S component field distributions are shifted towards stronger fields with regard to the IEFDF. In contrast, the F component FDFs are shifted towards smaller fields. The same occurs for the standard model whose most probable slow field is decreased due to the Debye screening term. In summary, in average F fields are stronger than S fields for the standard model. The opposite is found with ab initio methods implying that the balance between the S and F fields results drastically different for the present and the standard models. The unexpectedly large magnitude of the observed differences of the FDFs should be interpreted as a warning in favor of a careful use of the S and F components concepts, for instance, in the context of Stark broadening of lines.

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