# Molecular dynamics calculations of the spectral density of electron density fluctuations

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The correlation function of density fluctuations in hydrogen plasma is calculated by a Molecular Dynamics (MD) method. The model is validated by comparison with analytical results for coherent and incoherent regimes. Although to reproduce the analytical results using MD numerical experiment is a challenging task in the case of interacting plasma particles, preliminary simulation results suggest the possibility to catch the essential physics starting from first principles. In perspective, MD has the potential to address plasma parameter regimes which are intractable by the analytical approach.

## 1. Introduction

The kinetic theory of plasmas, based on the Bogoliubov-Klimontovich theory of fluctuations [1-3], rests on two assumptions: **(i)** the separation of time scales for average (continuous) and fluctuating (particle discreteness) parts of all quantities (distribution function, density, field) **(ii)** the conceptual separation of the fluctuations into "natural" and "induced", the latter induced in a system of charged particles by the fluctuating field generated by the natural (or "source") fluctuations due to particle discreteness and present in any large system of particles. The natural fluctuations are random and not known so that the theory is formulated in terms of their correlators providing the theoretical expressions for their spectral density.

In our previous work [4], natural fluctuations, corresponding to non-interacting particles, have been investigated by a combination of analytical and Molecular Dynamics (MD) methods for both unmagnetized and magnetized plasmas.

In this work we report on the developments of the numerical method to enable study of full density correlator by including interaction between the charged particles. Preliminary results are discussed in the light of comparison with the well-known analytical results in the coherent regime.

## 2. Method of calculation

In Ref. [4] we have extended to plasma a technique based on the analysis of density correlations that had been successfully applied to neutral atomic gases [5]. This procedure allows to include electrostatic interactions between particles, so that full (natural and induced) fluctuations in plasma can be accounted for.

The correlation function of density fluctuations in the wave number and frequency domain, $S(k, \omega)$, is calculated by Fourier transforming and squaring the numerical density fluctuations which have been sampled at discrete space-time points by MD method in (**r**,**v**) space. This simulated discrete power spectrum is equivalent, within normalization factors, to the theoretical spectrum. Multiple independent runs have been performed and their results have been averaged. Such ensemble averaging of the results reduces the statistical noise and enables us to estimate the variance of the results.

The computational method applied in this work is a special implementation of molecular dynamics with Monte Carlo initial conditions. At the initial time t=0 the particle spatial coordinates $x_i$, $y_i$, $z_i$ are randomly distributed in the cubic simulation box of size L, by using uniformly distributed random numbers $\eta_i$ between 0 and 1, as following; $x_i=L\eta_{1i}$, $y_i=L\,\eta_{2i}$, $z_i=L\eta_{3i}$. The initial particle velocity is selected according to the Maxwell–Boltzmann distribution at the temperature T using a direct method of sampling. For this purpose, indicating $v_i$ as the velocity component along the i-direction, we set $v_i = (-2T \ln \zeta_1/m)^{1/2} \sin(2\pi\zeta_2)$, using two random numbers $\zeta_1$ and $\zeta_2$ uniformly distributed between 0 and 1.

Periodic boundary conditions are used to avoid effects due to the finite size of the simulation box and to mimic an infinite one.

The spatial cell width and the time step are smaller than the corresponding characteristic plasma

quantities. The number of time step in a single run and the box size is chosen to optimize the resolution of S(k,ω).

To ensure that the temperature is constant we have implemented a thermostat that equilibrates the system fixing its average temperature, and at the same time allowing it to fluctuate around this average value.

The thermostat is based on the introduction of a fictitious friction force $\mathbf{F}_i^{fri} = -\xi \mathbf{v}_i$ acting on each particle i, which is proportional to its velocity $\mathbf{v}_i$ by means of the friction coefficient ξ. In this way the time evolution of particle positions and momenta is given by the following equations of motion:

$$d\mathbf{r}_i / dt = \mathbf{v}_i ; \quad m_i \, d\mathbf{v}_i / dt = \mathbf{F}_i^{int} + \mathbf{F}_i^{fri} \qquad (1)$$

Here $m_i$ and $\mathbf{r}_i$ are the mass and the position of the i-th particle, respectively, while $\mathbf{F}_i^{int}$ is the total force acting on the i-th particle. The friction coefficient is

$$\xi = \xi_0 (T-T_0)/T_0, \qquad (2)$$

where $T_0$ is the desired temperature, T is the current temperature of the system as calculated from the kinetic energy, and $\xi_0$ is the friction constant.

At every time step, T is calculated:

- if $T > T_0$ then $\xi > 0$ and $\mathbf{F}_i^{fri} < 0$ whereby each particle slow its motion and the system cools;
- if $T = T_0$ then $\xi = 0$ and $\mathbf{F}_i^{fri} = 0$ whereby each particle doesn't change its state of motion and the temperature of the system remains constant;
- if $T < T_0$ then $\xi<0$ and $\mathbf{F}_i^{fri} > 0$ whereby each particle accelerates its motion and the system heats up.

In this way the friction forces cause T to relax towards the desired temperature $T_0$ with a rate due to the numerical value of $\xi_0$. If $\xi_0$ is too big the system ceases to move and remains 'frozen' instead of tending to the desired dynamic, on the other hand, if $\xi_0$ is too small the relaxation is not numerically efficient.

In order to capture the collective behavior of the ensemble of simulated particles, it is essential to limit the contribution of the binary collisions. To be computationally effective, we introduce a cutoff radius $r_c$, such that only collisions between particles whose distance is in the range $[\, r_c , r_c (\ln \Lambda)^{1/2}]$ are implemented. Here $\ln \Lambda = 4\pi n \lambda_d^3$ is the Coulomb logarithm, and $\lambda_d$ is the Debye length.

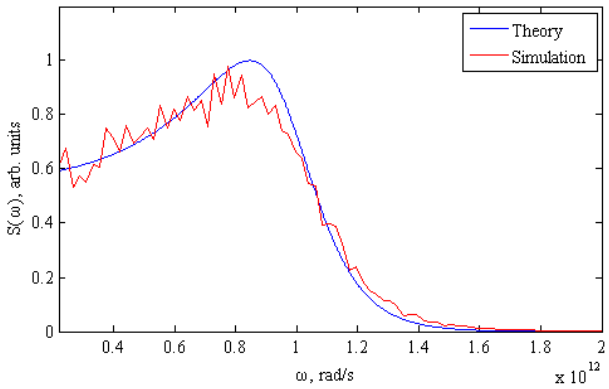


Fig.1 *Spectrum of electron density fluctuations S(k,ω) for $k=3.14\ 10^4\ m^{-1}$ and plasma parameters as specified in Sec.3.*

## 3. Results and conclusion

The simulations have been performed for Maxwellian electron and proton species at equal temperatures T = 1 keV and the number density of $n=10^{20}\ m^{-3}$, yielding $\lambda_d = 2.35\ 10^{-5}$ m and $\ln \Lambda = 4.08$.

To test coherent regime we aimed at k numbers which, for the plasma parameters chosen, yield a distinct weakly damped electron feature, for example, $k = 10^4\ m^{-1}$. To resolve such a case however implies to have box length of least $L = 2\pi/k = 628$ μm. With the available computational power, we have been able to perform runs with the total number of particles N=1000 which, for that the aforementioned L, limits the plasma parameter of *simulated* particles ($4\pi\lambda_d^3 N/3L^3$) to value of 0.22. In spite of this, the simulations have been able to reproduce an electron feature centered at the relevant for this k Langmuir wave frequency, even though significantly spread as compared to the theoretical predictions. Currently new runs are tested with increased number of particles which should increase the plasma parameter and, as we anticipate, to narrow the peak.

With nearly three times larger wave number, $k = 3.14\ 10^4\ m^{-1}$, yielding $k\lambda_d = 0.74$, we are not strictly in the coherent regime anymore. However this value allows us to benefit from nearly 30 times higher plasma parameter thanks to its scaling with $L^{-3}$. The results for this run are presented in Fig.1 and reveal quite reasonable agreement with the analytical theory. The reach similar agreement at lower frequencies requires significantly increased duration of the run which is currently being tested.

## 4. Outlook

Our final goal is to explore with the MD method developed here the parameter regimes inaccessible for analytical theory. These includes the environments where, for instance, the effects of neutrals and electron impact ionization, or the effects of Coulomb collisions and suprathermal particle sub-populations can play significant role, which we also aim to explore in parallel experimentally [6].

The focus of the current work is on validation of the method within regimes where analytical results are well established. Concerning the electron density fluctuations, thus far it appears that with an adequately increased computational power we shall be able to address the issue related to the plasma parameter and to reproduce the analytical results with acceptable accuracy.

## 5. References

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