Lecture no. 10

Transport Properties of Plasma by Molecular Dynamics Simulation

Introduction

In the previous lecture we have considered molecular dynamics method for computer simulation of equilibrium (thermodynamic) as well as non-equilibrium (transport) properties of plasma. Using this method the microscopic state (particle's coordinates, velocities etc.) can be obtained. But our final goal is the evaluation of transport properties of plasma such as diffusion, electrical conductivity, viscosity etc. For this purpose we will consider at first the autocorrelation functions of dynamical variables. Then we will show how can calculate macroscopic transport properties of plasma on the basis of the autocorrelation functions of microscopic dynamical variables.

Autocorrelation functions (ACF) of microscopic quantities. Properties of ACF

Definition. An autocorrelation function of random variable $X(t)$ is defined as follows:

$$G(S) = \left\langle X(t) \cdot X(t+S) \right\rangle, \tag{1}$$

where $\langle ... \rangle$ denotes the ensemble averaging. For random variable we have $\langle X \rangle = 0$. Thus an autocorrelation function at $S = 0$ has the following dispersion $\langle X^2 \rangle = 0$. **Autocorrelation function means the correlations between current and previous (or initial) microscopic states of the system.**

Properties of autocorrelation functions.

1) An autocorrelation function is the even one, i.e.

$$G(S) = G(-S)$$

2) An autocorrelation function has a maximum at $S = 0$. Actually,

$$\left\langle \left[X(t) \pm X(t+S) \right]^2 \right\rangle = \left\langle X^2(t) \right\rangle + \left\langle X^2(t+S) \right\rangle \pm 2 \left\langle X(t) X(t+S) \right\rangle \geq 0,$$

It follows that $G(0) \geq G(S)$.

3) Since $X(t)$ is a random quantity we can suppose that correlation between $X(t)$ and $X(t+S)$ is absent at large values of S, therefore:

$$\lim_{S\to\infty} G(S)=0$$

There are the most important autocorrelation functions for investigation of plasma's properties.

Velocity autocorrelation functions (VAF):

$$\langle \vec{\upsilon}(0)\vec{\upsilon}(t)\rangle = \frac{1}{3N}\sum_{i=1}^{N}\vec{\upsilon}_i(t_n)\cdot\vec{\upsilon}_i(t_n+t) \quad . \tag{2}$$

Microscopic electrical current correlation function:

$$\langle \vec{j}(0)\vec{j}(t)\rangle = \left\langle \sum_i Z_i\vec{\upsilon}_i(t)\cdot\sum_j Z_j\vec{\upsilon}_j(0)\right\rangle \tag{3}$$

For simplicity, autocorrelation functions are considered in units of

$$\sum_{i=1}^{N}\langle \vec{G}_i(0)\cdot\vec{G}_i(0)\rangle \quad . \tag{4}$$

In Figures 1 and 2 velocity autocorrelation functions and mean square displacements of coordinates of a dense semiclassical plasma are shown for different values of coupling parameter. It should be noted that fluctuations of these quantities lie within of statistical errors $\sim 1/\sqrt{N}$. The convergence of velocity autocorrelation functions becomes weak (slow) with decreasing of coupling parameter. This fact may be connected with decreasing of particle's collision frequency in weakly non-ideal plasma. Mean square displacements increase linearly up to value of dimensionless time (in units of the Longmuir frequency ω_e) $t\le 5$ according to the Einstein formula $\sim 6D(t-t_0)$. The saturation range ($t\ge 12$) indicates that particles are distributed uniformly and diffusion process reaches its stationary value.

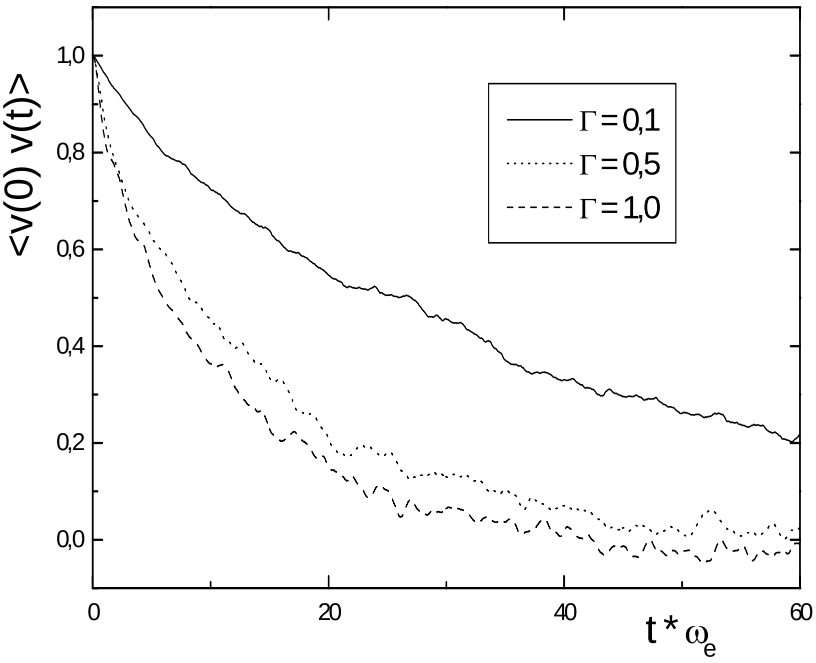

Figure 1. Dependences of velocity autocorrelation functions of dimensionless time at $r_S = 2$.

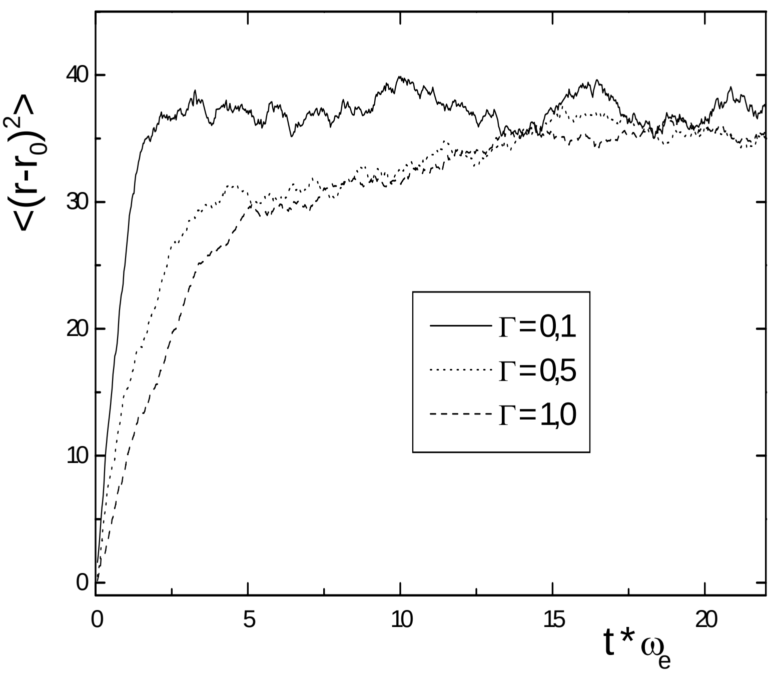

Figure 2. Mean square displacements of coordinates as a functions of dimensionless time at $r_S = 1$.

Relation between macroscopic (transport) coefficients and microscopic quantities in plasma. Basic principles of the Green-Kubo linear response theory

Using the microscopic states of the system we can estimate transport coefficients of plasma. For example, diffusion coefficient is calculated via mean square displacements of coordinates:

$$D = \lim_{t \to \infty} D(t) = \lim_{t \to \infty} \frac{\left\langle (\vec{r} - \vec{r}_0)^2 \right\rangle}{6(t - t_0)} . \quad (5)$$

In principal, knowing diffusion coefficient we can estimate another transport coefficients (for instance, by Onsager or Einstein relations).

Transport coefficients of plasma can be also obtained on the basis of the autocorrelation functions of microscopic dynamical variables. Relations between macroscopic (transport) coefficients and microscopic quantities in plasma are given by Green-Kubo linear response theory. According to this theory each macroscopic transport coefficient is defined by some microscopic dynamical variable (see, Table 1).

Table 1. The correspondence between microscopic dynamical variables and macroscopic transport coefficients of plasma

Dynamical variable	Transport coefficient
Velocity of particle - $\dot{\vec{r}}_i(t)$	Diffusion - D
Microscopic electric current $e\sum_i z_i \dot{\vec{r}}_i(t)$	Electrical conductivity - σ
Energy flux $\frac{d}{dt}\sum_i \vec{r}_i(t) E_i(t)$	Thermal conductivity - λ
Off-diagonal components of stress tensor $m\frac{d}{dt}\sum_i x_i(t)\dot{y}_i(t)$	Shear viscosity - η
Diagonal components of stress tensor $m\frac{d}{dt}\sum_i x_i(t)\dot{x}_i(t)$	Longitudinal viscosity $\frac{4\eta}{3} + \xi$

We can construct so-called Green-Kubo relations according to this table. For instance, diffusion coefficient is evaluated via velocity autocorrelation function as follows:

$$D = \frac{1}{3}\int_{0}^{\infty}\left\langle \vec{\upsilon}(0)\vec{\upsilon}(t)\right\rangle dt \quad . \tag{6}$$

An electrical conductivity is defined on the basis of the microscopic electrical current autocorrelation function by the following expression:

$$\sigma = const\int_{0}^{\infty}\left\langle \vec{j}(0)\,\vec{j}(t)\right\rangle dt \quad . \tag{7}$$

The basic principle of linear response theory for electrical conductivity of plasma can be explained as follows. Let plasma is located on the constant external electric field. Then in our system the electric current is induced, i.e. this current we can consider as a linear response to external perturbation (electric field). There is a direct proportionality between these quantities and they are related by well known Ohm's law:

$$\vec{j} = \sigma\vec{E} \quad , \tag{8}$$

where the proportionality coefficient σ is the electrical conductivity.

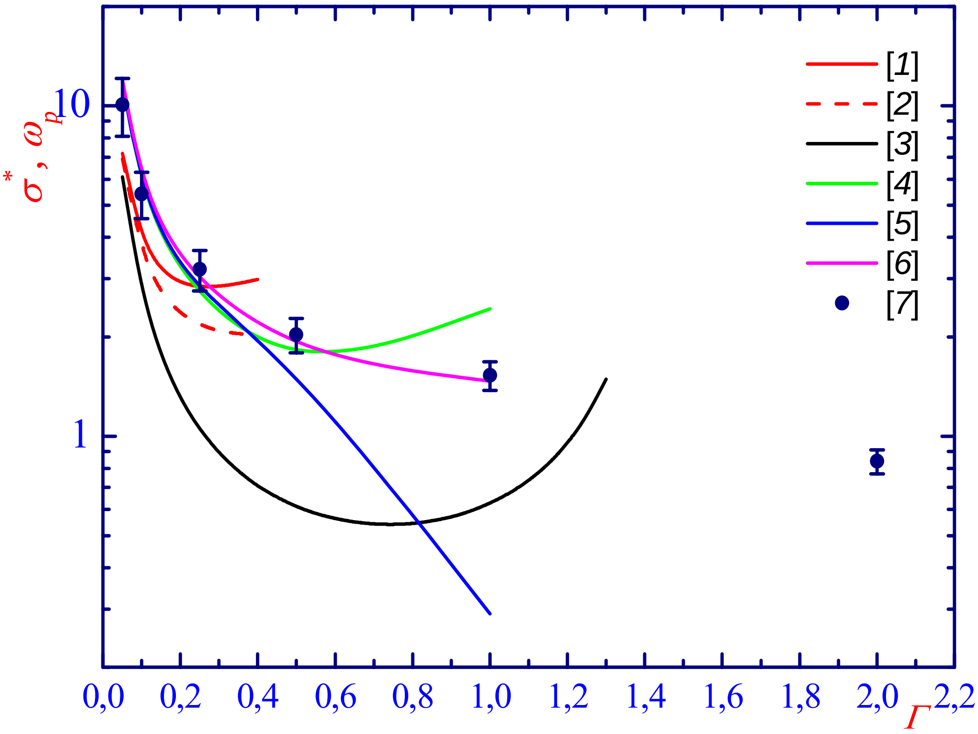

Figure 3. Electrical conductivity of nonideal hydrogen plasma.

[1], [2] T S Ramazanov, K N Dzhumagulova and A Zh Akbarov.//J. Phys. A: Math. Gen. **39** (2006) 4335.
[3] Spitzer theory
[4] Boercker D.B., Rogers F.J., DeWitt h.E.// Phys.Rev.A., 1982, v.25, p.1623.
[5] Baus Marc, Hansen Jean – Pierre, Sjogren Lenart. // Phys. Lett., V. 82A, № 4, 1980.
[6] Ishimaru S., Tanaka S.,// Phys. Rev., A.32, 1985, p. 1790.
[7] – T.S.Ramazanov, G.Nigmetova, G.Roepke, R.Redmer. // J.Plasma Phys. 2006.

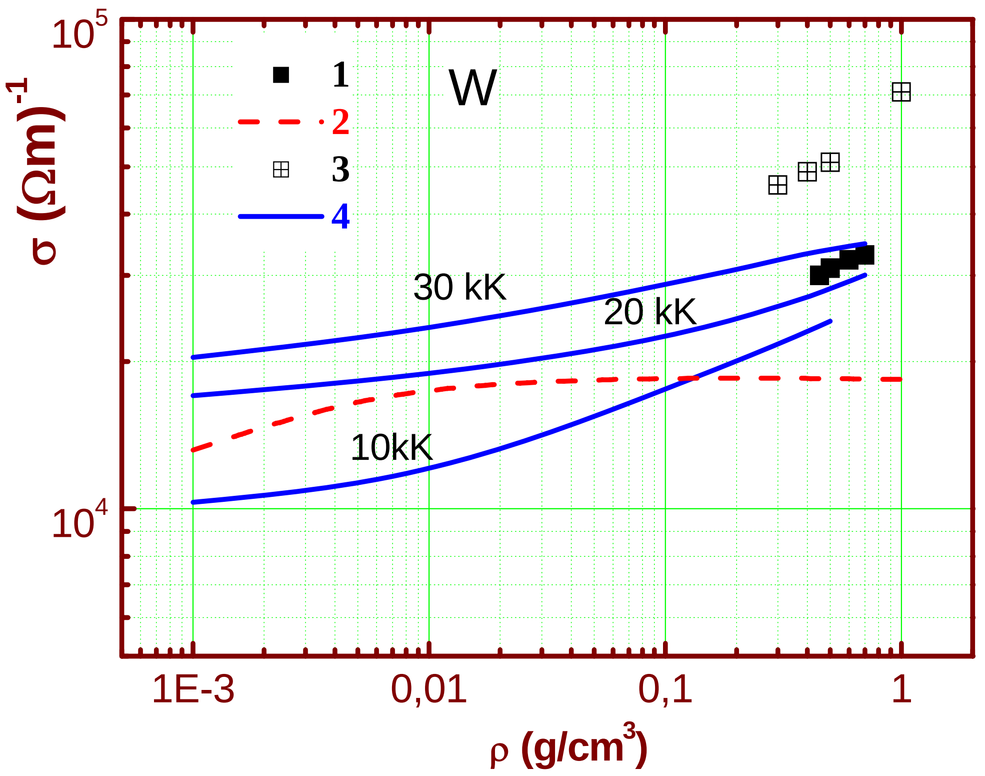

Figure 4. Electrical conductivity of nonideal tungsten plasma.

1 - Experiment: S.Saleem e.a., Phys. Rev.E. Vol.64. (056403)(2001) (for 20kK)

2 -Theoretical results for 20 kK of S.Kuhlbrodt, R.Redmer (Phys Rev. E – 2000. – vol. 62.)

3 -Y.T.Lee and R.M.Moore.(Phys. Fluids 27, 1273 (1984))

4 - Present work for different temperatures (T.Ramazanov, K.Galiyev, 2003)