

# N-body Lyapunov exponent in strongly coupled plasmas

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## INTRODUCTION

For large departures from equilibrium thermal quantities can not be defined meaningfully and transport process is not merely regarded as relaxation to the thermal equilibrium. It is difficult to treat the transport process in strongly non equilibrium or very slow relaxation with the method of present statistical mechanics. But even in that case mechanical characteristic quantities can be defined strictly. For example, the Lyapunov exponent is one of mechanical quantities which is an index of sensitive dependence on initial conditions. We conjecture that the Lyapunov exponent in phase space can provide a useful window on microscopic evolution systems.

In the conference [April 24-28, 1995, 12th LIRPP in OSAKA, JAPAN], we reported the calculations of the Lyapunov exponent in classical one component plasmas for the Coulomb coupling constant of  $\Gamma=1\sim 200$ . Important results we got are as follows. In 3 dimensional Coulomb many body system, initial information of adjacent trajectories is lost, in other words this system is mixing and ergodic. The Lyapunov exponents were found to be proportional to  $\Gamma^{-2/5}$  for  $\Gamma=1\sim 160$ , have a large jump at  $\Gamma\sim 170$  and be proportional to  $\Gamma^{-5/4}$  for  $\Gamma>170$ . The states correspond to liquid phase, phase transition point, and solid phase, respectively. We found that the largest Lyapunov exponent has the close relation to transport process. The diffusion coefficient obeys the third power of the Lyapunov exponent in liquid phase.

In this paper, we examine the relation between the Lyapunov exponent and the diffusion coefficient for three different strongly coupled Coulomb systems; one-component plasma, (OCP), semi-quantum OCP, (QOCP), and semi quantum two component plasma (TCP) for  $0.1<\Gamma<10$ .

## SIMULATION METHOD AND RESULT

It is necessary for particle simulation of dense Coulomb system to calculate precisely Coulomb interactions among distant and close particles. We perform the NVE ( particle number, volume, total energy ) constant molecular dynamics simulation with the use of a 3-d particle code SCOPE. Particle-Particle Particle-Mesh method is used in the code to treat many particles, in which Coulomb forces among close particles are directly summed up and Particle-Mesh method is employed for the calculation of forces among distant particles. The system comprised 500 or 1000 charged particles in periodic cubic box. Newton's equation of motion is solved using a leap-frog technique which has the second order accuracy in time step.

A state of strongly coupled plasmas is determined only by the Coulomb coupling constant ( $\Gamma$ ) and the Fermi degeneracy ( $\theta$ ). We assume that ion charge number ( $Z$ ) is unit and ion temperature ( $T_i$ ) is equal to electron temperature ( $T_e$ ).

$$\Gamma \equiv \frac{e^2}{aT}, \quad \frac{4\pi}{3}a^3 \equiv \frac{1}{n} \equiv \frac{N}{V}, \quad \theta \equiv \frac{T}{\epsilon_f}, \quad \epsilon_f \equiv \frac{\hbar^2}{2m_e} (3\pi^2 n)^{2/3}, \quad (1)$$

where  $e$ ,  $T$ ,  $a$ ,  $n$ ,  $N$ ,  $V$ ,  $\epsilon_f$ ,  $m_e$  and  $\hbar$  are charge, temperature (thermal energy), electron sphere radius, number density, particle number, volume, Fermi energy, electron mass, the Plank constant divided by  $2\pi$ . Potential used in our simulation, which is called Deutsch potential, is as follows :

$$\mu_{\alpha\beta} \equiv \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}, \quad \lambda_{\alpha\beta} \equiv \frac{\hbar}{\sqrt{2\pi T \mu_{\alpha\beta}}} = \left( \frac{2^4}{3^4 \pi^5} \right)^{1/6} \sqrt{\frac{m_e}{\mu_{\alpha\beta}}} a \theta^{-1/2},$$

$$\frac{e\Phi_{\alpha\beta}}{T} \equiv \Gamma \left\{ \sigma_{\alpha}\sigma_{\beta} \left( \frac{a}{r} - \frac{a}{r} \exp \left[ -\frac{r}{\lambda_{\alpha\beta}} \right] \right) + \frac{\delta_{\alpha\beta}}{\Gamma} \exp \left[ -\frac{1}{\pi \ln 2} \left( \frac{r}{\lambda_{\alpha\beta}} \right)^2 \right] \right\}, \quad (2)$$

where  $\alpha$  and  $\beta$  devote species of charged particles,  $\lambda_{\alpha\beta}$  is the thermal de Broglie length,  $\sigma_j$  is a sign, 1 or -1, of  $j$  charged particle, and  $\delta_{\alpha\beta}$  is Kronecker's delta. The first term,  $r/a$ , is pure Coulomb potential, the second term arises from quantum diffraction effect and the third term takes care of symmetry. [C.Deutsh: Phys.Lett. A60, 317 (1977)]

## LYAPUNOV EXPONENT

We measured of the Lyapunov exponents with the re-scaled method for various strongly coupled plasmas: classical one component (OCP : pure Coulomb and uniform ion background), semi-quantum OCP (QOCP :  $\theta=1$ ), and semi-quantum two component plasma (TCP :  $\theta=1$ ). The mass ratio,  $m_j/m_e$ , is set to be unit. Important results are as follows. Figure 1 shows relation between the Lyapunov exponent and the diffusion coefficient in OCP, QOCP and TCP. The Lyapunov exponent and the diffusion coefficient are normalized by plasma frequency,  $\omega_p = (4\pi e^2/m_e)^{1/2}$ , and  $a^2\omega_p$ . The Lyapunov exponents decreases from 2 to 0.3 with increasing of the Coulomb coupling constant and the differences of the Lyapunov exponent for three models are within factor 2. The diffusion coefficients estimate with the gradients of the mean square deviations. The diffusion coefficient is proportional to the third power of the Lyapunov exponent in the region of  $\lambda/\omega_p < 1$  even in the different models. Although, the third power law is broken in the region of  $\lambda/\omega_p > 1$ . We conjecture that this result, the third power law, is universal for  $\lambda/\omega_p < 1$ .

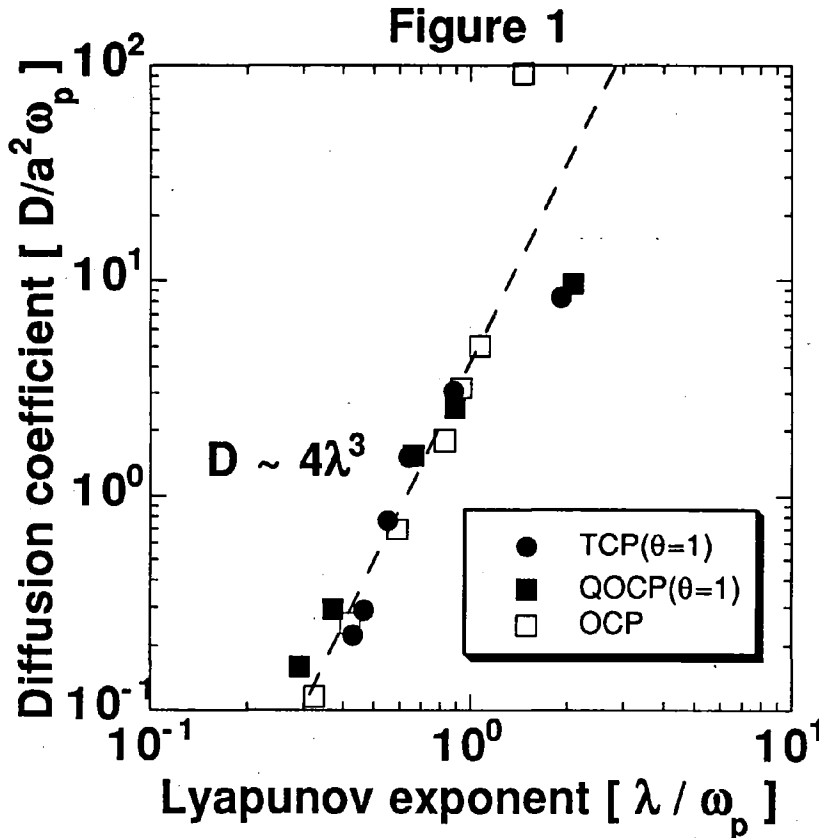


Fig. 1 This shows dependence of the diffusion coefficient on the Lyapunov exponent. Horizontal and perpendicular axes represent the Lyapunov exponent and the diffusion coefficient.