

Relation between Lyapunov Exponent and Dielectric Response Function in Dilute One Component Plasmas

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(Received 3 June 1996)

An analytical model is developed for the N -body largest Lyapunov exponent in the dilute plasma, and it is shown that the Lyapunov exponent relates to the dielectric response function. The relation provides a bridge between microscopic mechanical and macroscopic statistical quantities and it is expected to also be applicable for a weakly nonequilibrium system. In thermal equilibrium, the model shows that the Lyapunov exponent of dilute one component plasmas is of the same order as the plasma frequency and independent of the Coulomb coupling constant. These results agree fairly well with three dimensional particle simulations. [S0031-9007(97)04053-2]

PACS numbers: 05.45.+b, 02.50.Ey, 52.20.-j, 52.65.-y

Recently, there has been a great deal of research devoted to finding relations between the Lyapunov exponent and macroscopic statistical quantities [1–6]. The Lyapunov exponent is the rate at which knowledge of an initial state in phase space is lost. In previous works [1–3,5], systems that are determined only by short range forces and/or small degrees of freedom were mainly considered. In this paper, we consider a Coulomb many body system whose dynamics is determined by long range forces. In short range force systems, the Lyapunov exponent is expected to be proportional to the collision frequency [1]. The proportionality of the Lyapunov exponent to the collision frequency is obtained from the assumption that the interaction time is much shorter than an interval of collisions. In Coulomb systems the interaction time can be approximated by a duration that a particle with a thermal speed v_{th} ($T = mv_{th}^2$) travels a distance of a Debye length $\lambda_D \equiv \sqrt{T/4\pi ne^2}$ because the Coulomb force of individual particles is shielded beyond a Debye sphere, but not within a Debye sphere. Here e , m , n , and T represent charge and mass of a particle, number density, and temperature in energy units, respectively. In addition to this, within the duration a particle interacts with many surrounding particles of the order of $n\lambda_D^3$ which is very large in a dilute Coulomb system. Therefore, the Lyapunov exponent in the Coulomb many body system is expected to be different from that in short range force systems. We have investigated the dependence of the Lyapunov exponent on the Coulomb coupling constant of $\Gamma < 1$ with the use of the three dimensional particle code SCOPE [6,7]. As will be shown below, the magnitude of the Lyapunov exponent is found to be of the same order as the plasma frequency $\omega_p^{-1} = \lambda_D/v_{th}$ in this range, which is very large compared with the collision frequency for such dilute plasmas.

In the previous papers, many analytical formulas for the Lyapunov exponent were proposed. For example, Krylov [1] reported that the Lyapunov exponent is expected to be proportional to the collision frequency; Gaspard and Nico-

lis [2] related the diffusion coefficient of a Lorentz gas with its positive Lyapunov exponent and the Kolmogorov entropy; Seki *et al.* [3] and Barnett *et al.* [4] presented relations between the Lyapunov exponent and the diffusion coefficient; Chaudhuri *et al.* [5] found a formula for a driven nonlinear oscillator and related the Lyapunov exponent to a correlation of the second order derivative of the potential. We will also find a similar relation between the Lyapunov exponent and the second spatial derivative of the Coulomb potential for a many body system. We will then derive an analytical model which gives a relation between the Lyapunov exponent and the dielectric response function [8].

In this paper, we consider a one component plasma. The one component plasma is characterized only by the Coulomb coupling constant $\Gamma \equiv e^2/aT$, where a is the particle sphere radius, i.e., $4\pi a^3/3 \equiv 1/n$. In the case of $\Gamma \ll 1$, a plasma can be regarded as a dilute plasma, while a plasma with $\Gamma > 1$ is regarded as a strongly coupled plasma. Figure 1 shows the dependence of the Lyapunov

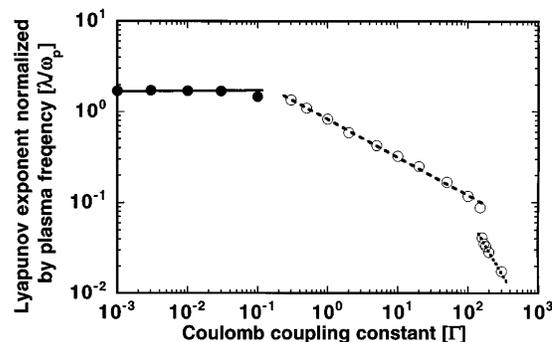


FIG. 1. Dependence of the Lyapunov exponents normalized by plasma frequency on the Coulomb coupling constant. Open and closed circles are data in the previous [4,6] and present works, respectively. Solid, broken, and dashed lines are obtained by a least-squares method with the observed data in the dilute, liquid, and solid plasmas, respectively.

exponents normalized by the plasma frequency on the Coulomb coupling constant Γ , obtained by molecular dynamics simulations using the three dimensional particle code SCOPE [6,7]. A Lyapunov exponent is defined in a long time limit as an exponential expansion rate of a separation distance between two adjacent trajectories in a $6N$ phase space. In the particle simulations, we consider two independent systems, reference and displaced systems, and both consist of 500 charged particles with uniform background charge and with a periodic boundary condition. In the displaced system, initial positions and momenta of the individual particles are displaced from their corresponding values in the reference system. The displacement is given by a normal distribution with the root mean squares of $5.0 \times 10^{-3} a$ in position coordinates and $5.0 \times 10^{-3} m v_{th}$ in the momentum space, respectively. The Lyapunov exponents in Fig. 1 are worked out by the conventional rescaled method [9], namely, by taking time average of the instantaneous expansion rates with respect to the displacement. The details of the simulation method are described in Ref. [6]. It is found that the Lyapunov exponent normalized by the plasma frequency, λ/ω_p , is independent of Γ for $\Gamma < 0.05$, proportional to $\Gamma^{-2/5}$ for $1 < \Gamma < 150$, and to $\Gamma^{-6/5}$ for $\Gamma > 170$. These states correspond to the dilute gas, dense liquid, and solid plasmas, respectively. The large jump of the Lyapunov exponent at $\Gamma \sim 170$ corresponds to the phase transition from liquid to solid state [10].

In the previous work [6], we explained qualitatively the simulation results of the dependence of the Lyapunov exponent on the Coulomb coupling constant in liquid and solid states on the analogy of a rigid body particle model and a weakly nonlinear lattice model, respectively. If the rigid body particle model [1,6] is applied for the dilute plasma, both the Lyapunov exponent and the collision frequency are expected to be proportional to $\omega_p \Gamma^{3/2}$. However, as shown in Fig. 1, for the dilute plasma ($\Gamma \leq 1$) the magnitude of the Lyapunov exponent is of the same order as the plasma frequency, namely, much larger than the collision frequency.

To construct a model for the Lyapunov exponent, we derive basic equations for the trajectory instability in the one component plasma. A classical three dimensional system of N particles has $3N$ momenta, \mathbf{p} , and $3N$ position coordinates \mathbf{q} . $\Lambda(\mathbf{p}, \mathbf{q})$ represents a $6N$ -dimensional phase space point. In the one component plasma, particle motion can be described with a Hamiltonian H as follows:

$$\dot{\Lambda} \equiv \begin{pmatrix} \dot{\mathbf{p}} \\ \dot{\mathbf{q}} \end{pmatrix} = \begin{pmatrix} -\partial H/\partial \mathbf{q} \\ \partial H/\partial \mathbf{p} \end{pmatrix} \equiv \mathbf{G}(\Lambda), \quad (1)$$

where

$$H = \sum_{i=1}^N \mathbf{p}_i^2/2m + \sum_{i=1}^N \sum_{j \neq i}^N e^2/2|\mathbf{q}_i - \mathbf{q}_j|$$

and the subscripts “ i ” and “ j ” denote, respectively, the i th and j th particles. To obtain the Lyapunov exponent, we need an equation of motion for a perturbed trajectory in the $6N$ phase space. Equation (1) is linearized as follows:

$$\begin{aligned} \dot{\delta} &\equiv \begin{pmatrix} \delta \dot{\mathbf{p}} \\ \delta \dot{\mathbf{q}} \end{pmatrix} = \frac{\partial \mathbf{G}(\Lambda)}{\partial \Lambda} \delta = \begin{pmatrix} \mathbf{0} & -\mathbf{V}_{\mathbf{q}, \mathbf{q}_j}(t) \\ \mathbf{m}^{-1} & \mathbf{0} \end{pmatrix} \delta \\ &\equiv \mathbf{T}(\Lambda) \delta, \end{aligned} \quad (2)$$

where

$$\mathbf{V}_{\mathbf{q}, \mathbf{q}_j}(t) \equiv \sigma_{ij} \sum_{\ell \neq i}^N \psi_{i\ell}(t) - (\mathbf{1} - \sigma_{ij}) \psi_{ij}(t)$$

and

$$\psi_{i\ell}(t) \equiv \partial^2(e^2/|\mathbf{q}_i(t) - \mathbf{q}_\ell(t)|)/\partial \mathbf{q}_i \partial \mathbf{q}_\ell.$$

In Eq. (2), $\delta \mathbf{p}$ and $\delta \mathbf{q}$ are the perturbed $3N$ -dimensional momentum and position coordinate, respectively, and σ_{ij} , \mathbf{m}^{-1} , and $\mathbf{0}$ are Kronecker's delta, diagonal tensor whose components are m^{-1} , and zero matrix, respectively. $\psi_{i\ell}$ represents the second order spatial derivative of the Coulomb potential induced by the ℓ th particles. Thus, $\sum_{\ell \neq i} \psi_{i\ell} \delta \mathbf{q}_i$ presents the difference of forces on the i th particle and a fictitious particle at nearby position of which distance from the i th particle is $\delta \mathbf{q}_i$. This difference of the forces determines the expansion speed of the nearby trajectories, i.e., Lyapunov exponent. In a short range force system, the difference of the acceleration appears only at the time when collision takes place, and no acceleration on particles at an interval of collisions. Thus it is believed that the Lyapunov exponent is related to collision frequency. However, in a dilute plasma, because of a long range force of the Coulomb interaction, the difference of the acceleration appears even at an interval of collisions along a nearly ballistic trajectory. Namely, thermal fluctuations of surrounding particles within a Debye sphere may cause a difference of the acceleration on the particles.

The largest Lyapunov exponent is defined as the maximum eigenvalue of the time dependent matrix $\mathbf{T}(\Lambda)$ in Eq. (2). However, the matrix elements are functions of time and as a result the Lyapunov exponent cannot be directly calculated from Eq. (2). The treatment of van Kampen [11] for stochastic differential equations is adopted to solve Eq. (2). Namely, $\mathbf{V}_{\mathbf{q}\mathbf{q}}$ is assumed to have a finite autocorrelation time τ_c , in the sense that for any two time points t_1 and t_2 such that $|t_2 - t_1| > \tau_c$, $\mathbf{V}_{\mathbf{q}\mathbf{q}}(t_1)$ is statistically independent of $\mathbf{V}_{\mathbf{q}\mathbf{q}}(t_2)$. We also introduce a statistical averaged δ with respect to the zeroth order trajectories which satisfy Eq. (1). The time derivative of the statistical averaged δ is then given by $\langle \dot{\delta}_i \rangle = \sum_j \langle \bar{\mathbf{T}}_{ij} \rangle \langle \delta_j \rangle$, where

$$\langle \bar{\mathbf{T}}_{ij} \rangle = \left(- \int_0^\infty d\tau \left(\frac{\tau}{m} \right)^2 \left\langle \sum_{\ell=1}^N \mathbf{V}_{\mathbf{q}, \mathbf{q}_\ell}(0) \mathbf{V}_{\mathbf{q}, \mathbf{q}_j}(-\tau) \right\rangle \begin{matrix} \mathbf{m}^{-1} \\ \mathbf{0} \end{matrix} \int_0^\infty d\tau \frac{\tau}{m} \left\langle \sum_{\ell=1}^N \mathbf{V}_{\mathbf{q}, \mathbf{q}_\ell}(0) \mathbf{V}_{\mathbf{q}, \mathbf{q}_j}(-\tau) \right\rangle \right), \quad (3)$$

and the bracket denotes an ensemble average. In general the leading term of the matrix elements is given by the integrated time-correlation function of $\mathbf{V}_{\mathbf{q},\mathbf{q}_\ell}$ in a form of $\int_0^\infty d\tau \langle \sum \mathbf{V}_{\mathbf{q},\mathbf{q}_\ell}(0) \mathbf{V}_{\mathbf{q},\mathbf{q}_\ell}(-\tau) \rangle$ [11]. It should be noted, however, that only the potential of $|\mathbf{q}_i - \mathbf{q}_j|^{-1}$, such as Coulomb and gravity potentials, results in the first order moment with respect to time as the leading term as shown in Eq. (3).

We can reduce the rank of the matrix $\langle \bar{\mathbf{T}}_{ij} \rangle$ by assuming that the correlation time between $\mathbf{V}_{\mathbf{q},\mathbf{q}_\ell}(0)$ and $\mathbf{V}_{\mathbf{q},\mathbf{q}_\ell}(-\tau)$ for $j \neq i$ in Eq. (3) is much shorter than that for $j = i$. The cross terms $\sum_{j \neq i} \langle \bar{\mathbf{T}}_{ij} \rangle \langle \delta_j \rangle$ can then be neglected. This assumption can be verified at least for the dilute plasma. The calculation $\langle \dot{\delta}_i \rangle = \sum_j \langle \bar{\mathbf{T}}_{ij} \rangle \langle \delta_j \rangle$ is then approximated to $\langle \dot{\delta}_i \rangle = \langle \bar{\mathbf{T}}_{ii} \rangle \langle \delta_i \rangle$.

In the matrix of $\langle \bar{\mathbf{T}}_{ii} \rangle$, the upper left element c_{11} and the upper right element c_{12} are the second and first order moments with respect to time, respectively. Since the autocorrelation time τ_c is short for the dilute plasmas, c_{11} is small compared with $\sqrt{c_{12}/m}$, as will be confirmed later. Then, the largest Lyapunov exponent is approximated to be $\lambda \sim \sqrt{c_{12}/m}$. For the sake of convenience for calculation, we divide the element c_{12} into two terms, $c_{12} = c_{121} + c_{122}$, where

$$\begin{aligned} \frac{c_{121}}{m} &\equiv \int_0^\infty d\tau \frac{\tau}{3m^2} \text{Tr} \left\langle \sum_{\ell \neq i}^N \psi_{i\ell}(0) \psi_{i\ell}(-\tau) \right\rangle, \\ \frac{c_{122}}{m} &\equiv \int_0^\infty d\tau \frac{\tau}{3m^2} \text{Tr} \left\langle \sum_{\ell \neq i}^N \psi_{i\ell}(0) \sum_{\ell \neq i}^N \psi_{i\ell}(-\tau) \right\rangle, \end{aligned} \quad (4)$$

where the factor of $\frac{1}{3}$ comes from the assumption of an isotropic system. From the definition of $\psi_{i\ell}$, as discussed

$$\begin{aligned} c_{121} &= (N-1) \int_0^\infty d\tau \frac{\tau}{3m} \int \int d^3\mathbf{p}_i d^3\mathbf{p}_\ell f(\mathbf{p}_i) f(\mathbf{p}_\ell) \\ &\quad \times \left(\frac{n}{N} \right)^2 \int \int d^3\mathbf{q}_i d^3\mathbf{q}_\ell \frac{(4\pi e^2)^2}{(2\pi)^6} \int \int d^3\mathbf{k}_0 d^3\mathbf{k}_\tau \frac{(\mathbf{k}_0 \cdot \mathbf{k}_\tau)^2}{k_0^2 k_\tau^2} e^{i(\mathbf{k}_0 + \mathbf{k}_\tau)(\mathbf{q}_i - \mathbf{q}_\ell)} e^{-i\mathbf{k}_\tau(\mathbf{p}_i - \mathbf{p}_\ell)\tau/m}. \end{aligned} \quad (5)$$

Integrating Eq. (5) in the following order, with respect to position coordinates (\mathbf{q}_i and \mathbf{q}_ℓ), momentum (\mathbf{p}_i and \mathbf{p}_ℓ), and time (τ), Eq. (5) can be written as follows:

$$\begin{aligned} \frac{c_{121}}{m} &= \left(\frac{\omega_p}{3\pi} \right)^2 \int_0^\infty (ka)^2 d(ka) \\ &\quad \times \int_0^\infty \frac{d\tau}{\tau} \left\{ \int_{-\infty}^\infty \frac{d\omega}{\omega_p} \text{Re}[\varepsilon(k, \omega) - 1] e^{i\omega\tau} \right\}^2, \end{aligned} \quad (6)$$

where $\varepsilon(k, \omega)$ is the dielectric response function and we have used the following relation in the integration:

$$\begin{aligned} \int_{-\infty}^\infty d\mathbf{p}^3 f(\mathbf{p}) e^{ik(\mathbf{p}/m)\tau} &= \frac{1}{2\omega_p^2 \tau} \int_{-\infty}^\infty d\tau \\ &\quad \times \{ \varepsilon(k, \omega) - 1 \} e^{-i\omega\tau}. \end{aligned} \quad (7)$$

Since the term c_{122} has the product of two summations over ℓ in Eq. (4), the ensemble average cannot be exchanged with the summation. However, since the second

before, Eq. (4) indicates that the Lyapunov exponent is given by the square root of the first moment with respect to time for the autocorrelation function of the acceleration difference. The terms c_{121} and c_{122} are similar, but since $\psi_{i\ell} = \psi_{\ell i}$, the term c_{122} consists of $\sum_{\ell \neq i} \psi_{i\ell}(0) \psi_{i\ell}(-\tau)$ and $\sum_{\ell_1 \neq i} (\psi_{i\ell_1}(0) \sum_{\ell_2 \neq i, \ell_1} \psi_{i\ell_2}(-\tau))$. The correlation between $\psi_{i\ell_1}$ and $\psi_{i\ell_2}$ ($\ell_2 \neq \ell_1$) cannot be neglected even for the dilute plasma. In fact, it will be shown that $c_{122} = 2c_{121}$ at least in thermal equilibrium systems. The time correlations in c_{121} and c_{122} are calculated by assuming a ballistic motion $\mathbf{q}_i(-\tau) = \mathbf{q}_i(0) - \mathbf{p}_i(0)\tau/m$ as the zeroth order trajectory. This assumption might be valid for the dilute plasma because the collisions are rare.

First, we derive a formula of the Lyapunov exponent as a function of the dielectric response function. The terms c_{121} and c_{122} are calculated in different ways. From the assumption of the ballistic motion, $\psi_{i\ell}(-\tau)$ can be written as

$$\begin{aligned} \psi_{i\ell}(-\tau) &= (2\pi)^{-3} (4\pi e^2) \int \int d^3\mathbf{k}_\tau (\mathbf{k}_\tau \mathbf{k}_\tau / k_\tau^2) \\ &\quad \times e^{i\mathbf{k}_\tau(\mathbf{q}_i - \mathbf{q}_\ell)} \\ &\quad \times e^{-i\mathbf{k}_\tau(\mathbf{p}_i - \mathbf{p}_\ell)\tau/m} \end{aligned}$$

through the Fourier transformation. Since each particle cannot be distinguished, the summation with respect to " ℓ " and ensemble average can be exchanged and the summation $\sum_{\ell \neq i}$ is replaced by $(N-1)$. The ensemble average with respect to the zeroth order trajectories of the i th and ℓ th particles are obtained by multiplying momentum distribution functions $f(\mathbf{p})$ and taking the average with respect to momentum and position coordinates. The term c_{121} can then be approximated as

order spatial derivative of potential is related to the charge density fluctuation, $\delta n(\mathbf{q}, t) \equiv \sum \delta(\mathbf{q} - \mathbf{q}_i(t)) - n$, through the Poisson equation, the correlation of $\sum_{\ell \neq i} \psi_{i\ell}$ can be replaced by that of the density fluctuations,

$$\begin{aligned} \text{Tr} \left\langle \sum_{\ell \neq i}^N \psi_{i\ell}(0) \sum_{\ell \neq i}^N \psi_{i\ell}(-\tau) \right\rangle &= (4\pi e^2)^2 \\ &\quad \times \langle \delta n(\mathbf{q}(0), 0) \\ &\quad \times \delta n(\mathbf{q}(-\tau), -\tau) \rangle. \end{aligned}$$

The space-time correlation of the density fluctuation should be taken along the trajectory of a particle. In a similar way as we derived Eq. (5), assuming ballistic motion, the term c_{122} can be expressed as

$$\begin{aligned} c_{122} &= \frac{(4\pi e^2)^2}{3(2\pi)^3} \int_0^\infty d\tau \frac{\tau}{m} \int_{-\infty}^\infty d\mathbf{p}^3 f(\mathbf{p}) \int_{-\infty}^\infty d\mathbf{k}^3 \\ &\quad \times \int_{-\infty}^\infty d\omega S(\mathbf{k}, \omega) e^{i(k(\mathbf{p}/m) - \omega)\tau}, \end{aligned} \quad (8)$$

where

$$S(\mathbf{k}, \omega) \equiv \int_{-\infty}^{\infty} d\mathbf{q}^3 dt \langle \delta n(0, 0) \delta n(\mathbf{q}, t) \rangle e^{-i(\mathbf{k} \cdot \mathbf{q} - \omega)t} / 2\pi$$

is the dynamic form factor which represents the power spectrum of the density fluctuations. The dynamic form factor is related to the dielectric response function $\varepsilon(k, \omega)$ through the fluctuation-dissipation theorem [8]. Using the fluctuation-dissipation theorem and the integration with respect to momentum Eq. (7), the term c_{122} can be expressed as

$$\frac{c_{122}}{m} = 2 \left(\frac{\omega_p}{3\pi} \right)^2 \left(\frac{\lambda_D}{a} \right)^2 \int_0^{\infty} (ka)^4 d(ka) \times \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \frac{\text{Im}[\varepsilon(k, \omega)] \text{Re}[\varepsilon(k, \omega) - 1]}{|\varepsilon(k, \omega)|^2}. \quad (9)$$

By using Eqs. (6) and (9), the Lyapunov exponent $\lambda = \sqrt{(c_{121} + c_{122})/m}$ can be calculated. It is thus shown that the N -body largest Lyapunov exponent generally related to the dielectric response function, although the relation contains the integration with respect to k , ω , and τ . The relation may be applicable for a weakly nonequilibrium system, wherein the dielectric response function is defined meaningfully. It should be noted that in Coulomb systems, the upper limit of the wave number in the integration in Eqs. (6) and (9) must be generally replaced by a certain finite value of k_{\max} to avoid meaningless divergence of the integration caused by lack of information of pair correlation for short range interaction.

Finally, let us estimate the Lyapunov exponent for a thermal equilibrium plasma from Eqs. (6) and (9). Using a Maxwellian distribution function in the relation of Eq. (7), Eq. (6) can be analytically integrated and written as follows:

$$\frac{c_{121}}{m} \sim \frac{8ne^4}{3m} \int_0^{k_{\max}} dk k^2 \int_0^{\infty} d\tau \frac{\tau}{m} \exp\left[-\frac{\tau}{\tau_0}\right]^2 = \frac{\omega_p^2 e^2}{3\pi T} \int_0^{k_{\max}} dk, \quad (10)$$

where $\tau_0 \equiv (k\sqrt{T/m})^{-1}$ represents the correlation time which depends on the wave number. In Eq. (9), the integration with respect to ω can be calculated by using the approximate formula of the plasma dispersion function [12] for its small and large arguments $Z \equiv (k\lambda_D)^{-1}(\omega/\omega_p)$. The leading term arises from small Z and Eq. (9) can then be approximated as follows:

$$\frac{c_{122}}{m} \sim 4 \left(\frac{\omega_p}{3\pi} \right)^2 \left(\frac{\lambda_D}{a} \right)^2 \int_0^{k_{\max}} (ka)^4 d(ka) \times \int_0^{\infty} \sqrt{\frac{\pi}{2}} \{1 + (k\lambda_D)^2\}^{-2} e^{-\frac{z^2}{2}} dZ \sim \frac{2\omega_p^2 e^2}{3\pi T} \int_0^{k_{\max}} dk. \quad (11)$$

Since the Landau length $e^2/T = a\Gamma$ [8] in the dilute plasma gives the closest distance that two particles can approach with repulsive Coulomb force, the maximum wave number may be approximated by a reciprocal of Landau length. Substituting $k_{\max} = 2\pi/a\Gamma$ in the terms c_{121} and c_{122} , we obtain $c_{121}/m = \omega_p^2 \Gamma a k_{\max} / 3\pi = 2\omega_p^2/3$ and $c_{122}/m = 2\omega_p^2 \Gamma a k_{\max} / 3\pi = 4\omega_p^2/3$. The element c_{11} is calculated in the same way as the element c_{12} . It is found that the element c_{11} is proportional to $\Gamma^{3/2} \ln(1/\Gamma)$ and thus c_{11} can be neglected in the dilute plasma. As a result, $\lambda = \sqrt{c_{122}/m} = \sqrt{2} \omega_p$ is obtained. The estimation indicates that the Lyapunov exponent is of the order of the plasma frequency.

In summary, we have constructed an analytical model for the largest Lyapunov exponent in the dilute plasma limit. The model indicates that the Lyapunov exponent is of the same order as the plasma frequency and is independent of the Coulomb coupling constant. The result is in good agreement with simulation data for the dilute plasmas. We have also shown that the Lyapunov exponent relates to the dielectric response function through the integration with respect to k , ω , and τ .

We thank Dr. M. Murakami, Dr. J. G. Wouchuk, and Dr. R. Ishizaki for useful comments. We also thank Professor K. Mima and Professor S. Nakai for their interest and encouragement throughout this work.

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