Lyapunov Exponent of a Many Body System and Its Transport Coefficients

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An *ab initio* theoretical expression for the N-body Lyapunov exponent of a dilute gas is derived. It shows the Lyapunov exponent to be a function of the time integral of the correlation function for the second derivative of the interparticle potential (approximately a power $\frac{1}{3}$ law). This establishes a link between the Lyapunov exponent and the transport coefficients. We compare the theory with numerical simulations of a one component plasma.

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The Gibbs ensemble in statistical mechanics serves as a microscopic formulation of equilibrium thermodynamics, and the fluctuation-dissipation theorem provides a microscopic connection to the system response functions and transport coefficients which characterize small departures from equilibrium. Far from equilibrium, Lyapunov expansion is a property with the potential to provide a useful microscopic description, when local definitions of quasi-equilibrium quantities, such as temperature and pressure, may no longer have meaning. The Lyapunov exponent measures the rate at which a system "forgets" its initial conditions. The transport coefficients are those response functions of the system that also measure a "forgetting." For example, scattering erases a particle's memory of its original velocity and so give rise to a finite diffusion coefficient. The work reported here creates an *ab initio* N-body microscopic theory of the microscopic Lyapunov exponent and gives an explicit functional relationship to a correlation function, in the limit of thermal equilibrium. We compare the theory with the numerical simulation of a one component plasma by Nishihara *et al.* [1,2].

A classical system of N particles in three dimensions has $3N$-dimensional vectors $\boldsymbol{p}$ and $\boldsymbol{q}$, respectively. We may represent these by a phase point, $\mathbf{\Upsilon} \equiv \binom{\boldsymbol{p}}{\boldsymbol{q}}$, in $6N$-dimensional phase space. For simplicity, we shall assume the particles have unit mass and a Hamiltonian of the form $H = \frac{1}{2}\boldsymbol{p} \cdot \boldsymbol{p} + V(\boldsymbol{q})$. Hamilton's equations of motion for the system are

$$\dot{\mathbf{\Upsilon}} \equiv \begin{pmatrix} \dot{\boldsymbol{p}} \\ \dot{\boldsymbol{q}} \end{pmatrix} = \begin{pmatrix} -V_{\boldsymbol{q}} \\ \boldsymbol{p} \end{pmatrix} \equiv \boldsymbol{G}(\mathbf{\Upsilon}), \tag{1}$$

where the notation $V_{\boldsymbol{q}}$ means the $3N$ gradient in the coordinates, $\partial V/\partial \boldsymbol{q}$. The detailed evolution of a system of interacting particles is, typically, very sensitive to changes in initial conditions. The Lyapunov exponent quantifies this sensitivity as follows. Consider a reference trajectory whose phase space point at time t is $\mathbf{\Upsilon}(t)$. At time $t = 0$ let another identical system be started which is infinitesimally displaced from the reference trajectory by $\mathbf{\Delta}(0)$. This displaced trajectory will evolve in time to $\mathbf{\Upsilon}(t) + \mathbf{\Delta}(t)$. Since $\mathbf{\Delta}(t)$ is infinitesimal, its equation of motion is given by the derivative of Hamilton's equation:

$$\dot{\mathbf{\Delta}}(t) = \frac{\partial \boldsymbol{G}(\mathbf{\Upsilon}(t))}{\partial \mathbf{\Upsilon}} \cdot \mathbf{\Delta}(t) \equiv \mathcal{T}(\mathbf{\Upsilon}(t)) \cdot \mathbf{\Delta}(t). \tag{2}$$

In sensitive systems, the displaced trajectory diverges from the reference system exponentially, on average. The mean exponential divergence rate is defined by [3]

$$\lambda(\mathbf{\Upsilon}(0), \mathbf{\Delta}(0)) = \lim_{\substack{t\to\infty \\ |\mathbf{\Delta}(0)|\to 0}} \frac{1}{t} \ln \frac{|\mathbf{\Delta}(t)|}{|\mathbf{\Delta}(0)|}. \tag{3}$$

The Lyapunov exponent $\lambda > 0$ and is independent of the direction of initial displacement $\mathbf{\Delta}(0)$ (unless it lies entirely in a special subspace which excludes the maximally expanding direction).

Other authors have sought analytic expressions for Lyapunov exponents of many body systems. Evans [4] has derived a short time formula to describe the mean separation of closely adjacent trajectories. The formula is based on a correlation in time, but lacks the time translation symmetry even in equilibrium. Chaudhuri, Gangopadhyay, and Ray [5] found a formula for a driven nonlinear oscillator (a system with one degree of freedom). It relates the Lyapunov exponent to a correlation in the second derivative of the potential. They reduce their equivalent of Eq. (2) to a simple harmonic oscillator with a stochastic frequency and apply the standard results of van Kampen [6].

Many authors have been exploring the connection between transport coefficients and Lyapunov exponents. Some examples are Gaspard and Nicolis [7] who find a connection between the diffusion coefficient of a Lorentz gas and its positive Lyapunov exponents and the Kolmogorov entropy; Evans, Cohen, and Morriss [8] who found a relation between viscosity and the maximum and

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minimum Lyapunov exponents which they computed for an upshifted Lennard-Jones potential in a nonequilibrium molecular dynamics simulation; and Chernov *et al.* [9] who proved, for a Lorentz gas, that Ohm's law entropy production is equal to minus the sum of the Lyapunov exponents. This paper presents an *ab initio* theory for the Lyapunov exponent of a many body system. An explicit form for a dilute gas, in the equilibrium limit, makes a connection with correlation functions and hence transport coefficients (via the fluctuation-dissipation theorem [10]).

We shall develop an equation of motion for the square infinitesimal distance, $|\mathbf{\Delta}(t)|^2$, between two adjacent trajectories in phase space. In order that the problem should remain linear we actually work with the outer product of $\mathbf{\Delta}(t)$ with itself, $[\mathbf{\Delta} \otimes \mathbf{\Delta}](t)$. The steps of our solution are as follows.

(1) Form the outer product of the displacement, $\mathbf{\Delta} \otimes \mathbf{\Delta}$ (a $6N \otimes 6N$ component entity).

(2) Solve the equation of motion

$$\frac{d}{dt}[\mathbf{\Delta} \otimes \mathbf{\Delta}](t) = \mathbb{T}(t) \cdot [\mathbf{\Delta} \otimes \mathbf{\Delta}](t), \tag{4}$$

where $\mathbb{T} \equiv \mathcal{T} \otimes \mathbf{1} + \mathbf{1} \otimes \mathcal{T}$ is the fourth rank, outer product version of the stability matrix appearing in Eq. (2). $\mathbb{T}(t)$ is shorthand for $\mathbb{T}(\mathbf{\Upsilon}(t))$, the t dependence being through the reference trajectory $\mathbf{\Upsilon}(t)$. The solution of Eq. (4) is formally a time-ordered exponential,

$$[\mathbf{\Delta} \otimes \mathbf{\Delta}](t) = \exp_T\left(\int_0^t d\tau\, \mathbb{T}(\tau)\right) \cdot [\mathbf{\Delta} \otimes \mathbf{\Delta}](0). \tag{5}$$

(3) Average Eq. (5) over an ensemble of reference trajectories and then differentiate to form a new differential equation for $\langle \mathbf{\Delta} \otimes \mathbf{\Delta} \rangle(t)$,

$$\frac{d}{dt}\langle \mathbf{\Delta} \otimes \mathbf{\Delta} \rangle(t) = \mathbb{L}(t) \cdot \langle \mathbf{\Delta} \otimes \mathbf{\Delta} \rangle(t). \tag{6}$$

(4) Evaluate $\mathbb{L}(\infty) = \lim_{t\to\infty} \mathbb{L}(t)$, since for large times $\mathbb{L}(t)$ should approach a constant value (i.e., forget the initial conditions).

(5) Find the eigenvalue ν of $\mathbb{L}(\infty)$ with the largest real part. Since $|\mathbf{\Delta}(t)|^2 = \mathrm{Tr}([\mathbf{\Delta} \otimes \mathbf{\Delta}](t))$, the Lyapunov exponent is

$$\lambda = \tfrac{1}{2} \max \mathrm{Re}(\nu). \tag{7}$$

The rules for operating with outer product operators are $[\mathcal{A} \otimes \mathcal{B}] \cdot [\mathcal{C} \otimes \mathcal{D}] \equiv [\mathcal{A} \cdot \mathcal{C}] \otimes [\mathcal{B} \cdot \mathcal{D}]$, and dot products $(\cdot)$ distribute over terms in a sum $(+)$.

We shall apply a standard perturbation technique [6,11] to evaluate $\mathbb{L}(\infty)$ to second order. In the dilute gas example, the zeroth and first order terms yield oscillatory eigenvalues only. The second order term (which involves correlations) is essential to reveal Lyapunov expansion behavior. Let $\mathcal{T}(t) = \mathcal{T}_0 + \mathcal{T}_1(t)$, where $\mathcal{T}_0$ is time independent and $\mathcal{T}_1(t)$ varies in time through a reference trajectory drawn from an ensemble. Evaluating Eq. (6) formally to second order in $\mathcal{T}_1$ gives an asymptotic evolution equation [11,12],

$$\frac{d}{dt}\langle \mathbf{\Delta} \otimes \mathbf{\Delta} \rangle(t) \underset{t\to\infty}{=} \left[\mathbb{T}_0 + \langle \mathbb{T}_1(t) \rangle + \int_0^\infty d\tau \langle\!\langle \mathbb{T}_1(t) \cdot e^{\tau \mathbb{T}_0} \cdot \mathbb{T}_1(t-\tau) \cdot e^{-\tau \mathbb{T}_0} \rangle\!\rangle \right] \cdot \langle \mathbf{\Delta} \otimes \mathbf{\Delta} \rangle(t), \tag{8}$$

where $\langle\!\langle AB \rangle\!\rangle \equiv \langle [A - \langle A \rangle][B - \langle B \rangle] \rangle$ is the correlation of A and B. The three terms in the square brackets are, respectively, the zeroth, first, and second order terms in the perturbation expansion of $\mathbb{L}(\infty)$. We consider $\mathbb{T}_1(t)$ to be small when the Kubo number $\alpha \tau_c$ is small, where α is the rms magnitude of $\mathbb{T}_1(t)$ and τ_c is the characteristic autocorrelation decay time scale.

For a dilute gas with a Hamiltonian of the form $H = \frac{1}{2}\boldsymbol{p} \cdot \boldsymbol{p} + V(\boldsymbol{q})$, we partition the stability matrix $\mathcal{T}$ of Eq. (2) into a constant part $\mathcal{T}_0$ due to free particle ballistic motion and a time dependent perturbation $\mathcal{T}_1(t)$ due to particle interactions, where

$$\mathcal{T}_0 = \begin{pmatrix} 0 & 0 \\ \mathbf{1} & 0 \end{pmatrix} \quad \text{and} \quad \mathcal{T}_1(t) = \begin{pmatrix} 0 & -V_{\boldsymbol{qq}}(\boldsymbol{q}(t)) \\ 0 & 0 \end{pmatrix}. \tag{9}$$

The corresponding outer product operators are

$$\begin{aligned} \mathbb{T}_0 &= \mathcal{T}_0 \otimes \mathbf{1} + \mathbf{1} \otimes \mathcal{T}_0, \\ \mathbb{T}_1(t) &= \mathcal{T}_1(t) \otimes \mathbf{1} + \mathbf{1} \otimes \mathcal{T}_1(t). \end{aligned} \tag{10}$$

The first order term in Eq. (8) is simply

$$\langle \mathbb{T}_1(t) \rangle = \mathbf{1} \otimes \langle \mathcal{T}_1(t) \rangle + \langle \mathcal{T}_1(t) \rangle \otimes \mathbf{1}. \tag{11}$$

We evaluate the exponential factor of the second order term by

$$e^{\tau \mathbb{T}_0} = e^{\tau \mathcal{T}_0} \otimes e^{\tau \mathcal{T}_0}. \tag{12}$$

For ballistic motion, using Eq. (9), we have

$$e^{\tau \mathcal{T}_0} = \begin{pmatrix} 1 & 0 \\ \tau & 1 \end{pmatrix}. \tag{13}$$

In order to better understand the explicit form of the integrand in the second order term of Eq. (8), it is helpful to "flatten" the $6N \otimes 6N$ phase space outer product into a four-component column of $3N \otimes 3N$ outer products showing the momenta and positions explicitly:

$$\mathbf{\Delta} \otimes \mathbf{\Delta} \equiv \begin{pmatrix} \mathbf{\Delta}_p \otimes \mathbf{\Delta}_p \\ \mathbf{\Delta}_p \otimes \mathbf{\Delta}_q \\ \mathbf{\Delta}_q \otimes \mathbf{\Delta}_p \\ \mathbf{\Delta}_q \otimes \mathbf{\Delta}_q \end{pmatrix}. \tag{14}$$

In this representation the integrand in Eq. (8) becomes

$$\langle\!\langle \mathbb{T}_1(t)\cdot e^{\tau\mathbb{T}_0}\cdot\mathbb{T}_1(t-\tau)\cdot e^{-\tau\mathbb{T}_0}\rangle\!\rangle = \begin{pmatrix} -\tau^2\langle\!\langle \mathbb{V}_0\cdot\mathbb{V}_\tau+\mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau^{\mathrm{T}}\rangle\!\rangle & \tau\langle\!\langle \mathbb{V}_0\cdot\mathbb{V}_\tau-\mathbb{V}_0\cdot\mathbb{V}_\tau^{\mathrm{T}}\rangle\!\rangle & \tau\langle\!\langle \mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau^{\mathrm{T}}-\mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau\rangle\!\rangle & \langle\!\langle \mathbb{V}_0\cdot\mathbb{V}_\tau^{\mathrm{T}}+\mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau\rangle\!\rangle \\ \mathbf{0} & -\tau^2\langle\!\langle \mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau^{\mathrm{T}}\rangle\!\rangle & -\tau^2\langle\!\langle \mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau\rangle\!\rangle & \tau\langle\!\langle \mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau+\mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau^{\mathrm{T}}\rangle\!\rangle \\ \mathbf{0} & -\tau^2\langle\!\langle \mathbb{V}_0\cdot\mathbb{V}_\tau^{\mathrm{T}}\rangle\!\rangle & -\tau^2\langle\!\langle \mathbb{V}_0\cdot\mathbb{V}_\tau\rangle\!\rangle & \tau\langle\!\langle \mathbb{V}_0\cdot\mathbb{V}_\tau^{\mathrm{T}}+\mathbb{V}_0\cdot\mathbb{V}_\tau\rangle\!\rangle \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}, \tag{15}$$

where $\mathbb{V}_\tau \equiv \mathbf{1}\otimes V_{\boldsymbol{qq}}(\boldsymbol{q}(t-\tau))$ and its transpose is $\mathbb{V}_\tau^{\mathrm{T}} \equiv V_{\boldsymbol{qq}}(\boldsymbol{q}(t-\tau))\otimes\mathbf{1}$. The elements of the matrix in Eq. (15) have the structure of 1, τ, or τ^2 times a correlation function. The correlation functions are of two types,

$$\langle\!\langle \mathbb{V}_0\cdot\mathbb{V}_\tau\rangle\!\rangle = \mathbf{1}\otimes\langle\!\langle V_{\boldsymbol{qq}}(\boldsymbol{q}(t))\cdot V_{\boldsymbol{qq}}(\boldsymbol{q}(t-\tau))\rangle\!\rangle, \tag{16}$$

where the correlation itself has rank 2 and rank 4 terms of the form $\langle\!\langle \mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau\rangle\!\rangle$. It is important to note that $\boldsymbol{q}(t-\tau)$ is just an earlier point of the trajectory specified by $\boldsymbol{q}(t)$. The trace back in time must be done before averaging over the ensemble of $\{\boldsymbol{p}(t),\boldsymbol{q}(t)\}$, which define the reference trajectories.

The next step is to average over an ensemble of reference trajectories—equilibrium here—in order to show the relation to other statistical quantities. We shall use the following conventions: unsubscripted $\boldsymbol{p}$ and $\boldsymbol{q}$ will represent the $3N$-dimensional vectors of momenta and positions of all the particles. When we use subscripts, these will label the coordinates of a particular particle. For example, $\boldsymbol{p}_i$ is the three-momentum vector for particle i.

A dilute monatomic gas in equilibrium is, on average, both isotropic and time translation invariant. The time translation invariance allows us to replace t by 0 in Eqs. (11) and (15). The rotational isotropy applies to the 3×3 submatrices (labeled by pairs of particles, i and j) and $3\times 3\otimes 3\times 3$ fourth rank tensors of the form $\langle V_{\boldsymbol{q}_i\boldsymbol{q}_j}(0)\otimes V_{\boldsymbol{q}_k\boldsymbol{q}_l}(-\tau)\rangle$. Rotational averaging of tensors is treated in Appendix B of Barnett [12]. We shall assume that $V(\boldsymbol{q})$ can be expressed as a function of the $N(N-1)/2$ pair differences in particle coordinates, $\boldsymbol{q}_i-\boldsymbol{q}_j$. With this condition $V_{\boldsymbol{q}_i\boldsymbol{q}_j}$ is a symmetric matrix even when $i\neq j$.

In Eq. (11) the rotational isotropy simplifies each submatrix to

$$\langle V_{\boldsymbol{q}_i\boldsymbol{q}_j}(0)\rangle = \frac{1}{3}\langle \mathrm{Tr}[V_{\boldsymbol{q}_i\boldsymbol{q}_j}(0)]\rangle\mathbf{1} \equiv \omega_{ij}^2\mathbf{1}. \tag{17}$$

Similarly, each submatrix in Eq. (16) averages to

$$\langle\!\langle V_{\boldsymbol{qq}}(\boldsymbol{q}(0))\cdot V_{\boldsymbol{qq}}(\boldsymbol{q}(-\tau))\rangle\!\rangle_{ij} = \frac{1}{3}\sum_{k=1}^{N}\langle\!\langle \mathrm{Tr}[V_{\boldsymbol{q}_i\boldsymbol{q}_k}(\boldsymbol{q}(0))\cdot V_{\boldsymbol{q}_k\boldsymbol{q}_j}(\boldsymbol{q}(-\tau))]\rangle\!\rangle\mathbf{1} \equiv c_{ij}(\tau)\mathbf{1}. \tag{18}$$

Rotational averaging the fourth rank subtensor gives

$$\langle\!\langle \mathbb{V}_0^{\mathrm{T}}\cdot\mathbb{V}_\tau\rangle\!\rangle_{ijkl} = a_{ijkl}(\tau)\mathbb{I} + b_{ijkl}(\tau)\mathbb{J}, \tag{19}$$

where the $3\times 3\times 3\times 3$ tensors are $\mathbb{J}_{\alpha\beta\gamma\delta} = \delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma}$ and $\mathbb{I}\equiv\mathbf{1}\otimes\mathbf{1}$, and the coefficients, labeled by particles and τ, are

$$a_{ijkl}(\tau) = \frac{1}{15}[2\langle\!\langle \mathrm{Tr}\{V_{\boldsymbol{q}_i\boldsymbol{q}_j}(\boldsymbol{q}(0))\}\mathrm{Tr}\{V_{\boldsymbol{q}_k\boldsymbol{q}_l}(\boldsymbol{q}(-\tau))\}\rangle\!\rangle - \langle\!\langle \mathrm{Tr}\{V_{\boldsymbol{q}_i\boldsymbol{q}_j}(\boldsymbol{q}(0))\cdot V_{\boldsymbol{q}_k\boldsymbol{q}_l}(\boldsymbol{q}(-\tau))\}\rangle\!\rangle], \tag{20}$$

$$b_{ijkl}(\tau) = \frac{1}{30}[-\langle\!\langle \mathrm{Tr}\{V_{\boldsymbol{q}_i\boldsymbol{q}_j}(\boldsymbol{q}(0))\}\mathrm{Tr}\{V_{\boldsymbol{q}_k\boldsymbol{q}_l}(\boldsymbol{q}(-\tau))\}\rangle\!\rangle + 3\langle\!\langle \mathrm{Tr}\{V_{\boldsymbol{q}_i\boldsymbol{q}_j}(\boldsymbol{q}(0))\cdot V_{\boldsymbol{q}_k\boldsymbol{q}_l}(\boldsymbol{q}(-\tau))\}\rangle\!\rangle]. \tag{21}$$

To make further progress with the second order term we shall assume that the potential energy is particle pairwise additive and the pair interaction has finite range. Examples of such forces are Lennard-Jones and screened Coulomb. The finite range allows us to neglect contributions to the correlation average from neighbors outside a small interaction volume s. Under the dilute gas assumption we may neglect intrinsic three and four body correlations, that is, we may neglect correlations where the two particle pairs are not identical. Each particle pair contributes $O(sn/N)$ to the average, where n is the mean particle density. Discarding terms $O(1/N)$ leaves just ω_{ii}^2, $c_{ii}(\tau)$, $a_{iiii}(\tau)$, and $b_{iiii}(\tau)$. The same assumptions also give

$$c_{ii}(\tau) = 2[a_{iiii}(\tau)+4b_{iiii}(\tau)]. \tag{22}$$

With these simplifications, the differential equation, (8), decouples by particle.

The problem has reduced to finding the eigenvalues of a single particle block, which can be thought of as a 36×36 matrix. The problem further diagonalizes into nine 4×4 submatrices according to the eigendirections of the operator $\mathbb{J}$. The only eigendirection which can contribute to $\langle|\boldsymbol{\Delta}|^2\rangle$ has eigenvalue [12] $J=4$. Therefore the fourth rank coefficients will appear only in the combination $a_{iiii}(\tau)+4b_{iiii}(\tau) = \frac{1}{2}c_{ii}(\tau)$.

Adopting the notation

$$c_m \equiv \int_0^\infty d\tau\,\tau^m c_{ii}(\tau), \quad m=1,\ 2,\ \text{or}\ 3, \tag{23}$$

the resulting matrix whose eigenvalues we seek is

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -\omega_{ii}^2 & -\omega_{ii}^2 & 0 \\ 0 & 0 & 0 & -\omega_{ii}^2 \\ 0 & 0 & 0 & -\omega_{ii}^2 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} -2c_2 & \frac{1}{2}c_1 & \frac{1}{2}c_1 & c_0 \\ 0 & -c_2 & -\frac{1}{2}c_2 & \frac{3}{2}c_1 \\ 0 & -\frac{1}{2}c_2 & -c_2 & \frac{3}{2}c_1 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (24)$$

The eigenvalues ν are solutions of

$$[\nu + \tfrac{1}{2}c_2]\{\nu^3 + \tfrac{7}{2}c_2\nu^2 + [3c_2^2 - 4(c_1 - \omega_{ii}^2)]\nu - 6c_1c_2 - 2c_0\} = 0. \quad (25)$$

The Lyapunov exponent is $\lambda = \frac{1}{2}\max \mathrm{Re}(\nu)$. Typically, each gas particle finds itself in a cage formed by all the others. On average, it experiences a potential well whose bottom is at the center of the cage. Hence the second derivative sign implies $\omega_{ii}^2 \geq 0$, which, by itself, would make ν imaginary. (For the Coulomb force, $\omega_{ii}^2 = 0$.) In addition, if the autocorrelation time is short then c_0 dominates terms with c_1 or c_2 in Eq. (25). If we take this to be so then there is indeed a solution with positive $\mathrm{Re}(\nu)$, namely, $\nu = [2c_0]^{1/3}$. Hence the Lyapunov exponent for a dilute gas in equilibrium is given by

$$\lambda = \left[\frac{c_0}{4}\right]^{1/3} = \left[\frac{1}{6}\int_0^\infty d\tau \langle\!\langle \mathrm{Tr}[V_{\boldsymbol{q}_i\boldsymbol{q}_i}(0)\cdot V_{\boldsymbol{q}_i\boldsymbol{q}_i}(-\tau)]\rangle\!\rangle\right]^{1/3}. \quad (26)$$

Equation (26) shows the equilibrium Lyapunov exponent to be proportional to the cube root of the integral of an autocorrelation function of the fluctuations of a dynamical variable. The fluctuation-dissipation theorem [10,13] relates linear response functions to corresponding correlation integrals. The correlation in Eq. (26) is for a single particle property. The intensities and correlation time scales of different single particle properties may be expected to vary in the same way with changes in system parameters such as temperature and pressure. In particular, the diffusion coefficient is proportional to the time integral of a particle's velocity autocorrelation. This leads us to suggest that the Lyapunov exponent is proportional to the cube root of the diffusion coefficient. Nishihara *et al.* [1,2] have run simulations of a dense one-component plasma using SCOPE, a particle-particle particle-mesh code. They measured both the Lyapunov exponent and the self-diffusion coefficient for a range of plasma parameters. The plasma parameter is the ratio of mean potential energy to kinetic energy for the charged particles. The results, plotted in Fig. 1, clearly show a one-third power dependence of the Lyapunov exponent on the diffusion coefficient over nearly three decades of diffusion data.

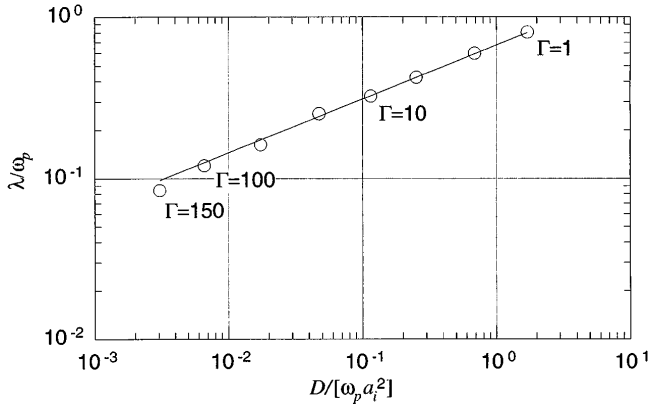

FIG. 1. Lyapunov exponent versus the diffusion coefficient for plasma parameter Γ values between 1 and 150. The data were computed by Nishihara *et al.* [1,2] for a one-component plasma. The line is $\lambda = aD^{1/3}$—the law suggested by the theory.

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