Fluctuations and the Many Body Lyapunov Exponent

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Abstract

An ab initio theoretical method is derived for calculating the maximal Lyapunov exponent of an N-body system obeying Hamilton's equations. The theory is developed in detail for a dilute gas. It shows the Lyapunov exponent to be a function of the time integral of the correlation function for fluctuations in the second derivative of the inter-particle potential (approximately a power $\frac{1}{3}$ law). We apply the theory to a one component plasma and derive the dependence of the Lyapunov exponent on plasma parameter.

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1 Introduction

1.1 Motivation

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 potential to provide a useful microscopic description, when local definitions of quasi-equilibrium quantities, such as temperature and pressure, may no longer have meaning. To be useful, we must establish two things: a viable definition of Lyapunov expansion, local in phase space[1], and a rigorous connection between Lyapunov expansion and macroscopic properties of a system out of equilibrium. This paper makes the latter connection, in the near-equilibrium regime.

Intuitively, the connection is plausible. 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 gives rise to a finite self-diffusion coefficient[2].

The work reported here creates an *ab initio* N-body microscopic theory of the microscopic Lyapunov exponent. The method is quite general and in future work we shall apply it to anharmonic crystals. Here we develop the theory for a

dilute gas or unmagnetized plasma. It gives an explicit functional relationship to a correlation function (a one third power law), in the limit of thermal equilibrium. Thus the Lyapunov exponent is related to system fluctuations. By way of detailed example, we applied the theory to a one component plasma. We have compared the theoretical predictions with a numerical simulation of the plasma, performed by Nishihara *et al.*[2–4] using SCOPE, a particle-particle particle-mesh program, adapted to compute the Lyapunov exponent.

1.2 Background

A classical system of N particles in 3 dimensions has $3N$ momenta and $3N$ position coordinates. We shall write them as the $3N$-dimensional vectors $\boldsymbol{p}$ and $\boldsymbol{q}$ respectively. We may represent these by a phase point, $\boldsymbol{\Upsilon} \equiv \begin{pmatrix} \boldsymbol{p} \\ \boldsymbol{q} \end{pmatrix}$, in $6N$-dimension 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

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

where the notation $V_{\boldsymbol{q}}$ means the $3N$-gradient in the coordinates, $\partial V/\partial \boldsymbol{q}$.

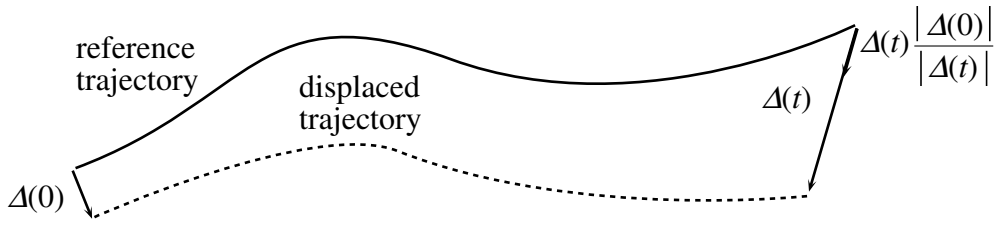

Figure 1: Displaced trajectory diverging from the reference trajectory

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 $\boldsymbol{\Upsilon}(t)$. At time $t = 0$ let another, identical system be started which is displaced infinitesimally from the reference trajectory by $\boldsymbol{\Delta}(0)$. This displaced trajectory will evolve in time to $\boldsymbol{\Upsilon}(t)+\boldsymbol{\Delta}(t)$, (see Figure 1). Since $\boldsymbol{\Delta}(t)$ is infinitesimal, its equation of motion is given by the derivative of Hamilton's equation:

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

In sensitive systems, the displaced trajectory diverges from the reference system exponentially, on average. The mean exponential divergence rate is defined by[5]

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

There is a $6N$-dimensional basis, $\{\hat{\boldsymbol{e}}_i\}$, of the $\boldsymbol{\Delta}(0)$, such that for any given $\boldsymbol{\Upsilon}(0)$, λ takes on one of the $6N$ (possibly non distinct) values

$$\lambda_i(\boldsymbol{\Delta}(0)) = \lambda_i(\boldsymbol{\Delta}(0), \hat{\boldsymbol{e}}_i) \tag{4}$$

These are the Lyapunov characteristic exponents. They can be ordered by size:

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{6N}. \tag{5}$$

Except for a set of measure zero, an arbitrary $\boldsymbol{\Delta}(0)$ will always have a component in the $\hat{\boldsymbol{e}}_1$ direction. If $\lambda_1 > 0$ then, in the limit $t \to \infty$, the largest exponent will dominate and adjacent trajectories will diverge exponentially at rate λ_1. This is

characteristic of sensitive dependence on initial conditions. In what follows we shall be dealing with the maximal Lyapunov exponent only and we shall drop the subscript; $\boldsymbol{\Delta}$ will refer to any particular initial displacement direction (almost all) which expresses the maximal Lyapunov exponent, λ.

Other authors have sought analytic expressions for Lyapunov exponents of many body systems. Evans[6] has derived a short time formula to describe the mean separation of close adjacent trajectories. The formula is based on a correlation in time, but lacks the time translation symmetry even in equilibrium. Chaudhuri et al.[7] 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 equation (2) to a simple harmonic oscillator with a stochastic frequency and apply the standard results of Van Kampen[8].

Many authors have been exploring the connection between transport coefficients and Lyapunov exponents. Some examples are: Gaspard and Nicolis[9] 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[10] found a conjugate pairing rule between maximum and minimum Lyapunov exponents and transport in non-equilibrium thermostatted molecular dynamics simulations, and illustrated it with a viscosity computation for particles interacting via an upshifted Lennard-Jones potential; entropy production as minus the sum of the Lyapunov exponents was noted by Hoover and Posch[11] and discussed by Evans and Morriss in their treatise[12]; and Chernov *et al.*[13] proved the sum rule for Ohm's law entropy production in a Lorentz gas.

Section 2 of this paper presents an *ab initio* theory for the Lyapunov exponent of a many body system obeying Hamilton's equations.. In Section 3, an explicit form for a dilute gas or plasma, in the equilibrium limit, makes a connection with correlation functions and hence transport coefficients (via the fluctuation-dissipation theorem[14]). The dilute gas exhibits a one-third power rule. Section 4 applies the theory, in detail, to a one component plasma.

2 Calculating the Lyapunov exponent *ab initio*

2.1 Exact method

We shall develop an equation of motion for the square infinitesimal distance, $|\boldsymbol{\Delta}(t)|^2$, between two adjacent trajectories in phase space. In order that the problem should remain linear we actually work with the outer product of $\boldsymbol{\Delta}(t)$ with itself, $[\boldsymbol{\Delta}\otimes\boldsymbol{\Delta}](t)$. Taking an ensemble average of the equation of motion gives a new equation for the evolution of $\langle\, \boldsymbol{\Delta}\otimes\boldsymbol{\Delta}\,\rangle(t)$. Asymptotically, $\langle\, \boldsymbol{\Delta}\otimes\boldsymbol{\Delta}\,\rangle(t)$, will expand at twice the Lyapunov rate. The steps of our solution are:

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

2. Solve the equation of motion,

$$\frac{d}{dt}[\boldsymbol{\Delta}\otimes\boldsymbol{\Delta}](t) = \mathbb{T}(t)\cdot[\boldsymbol{\Delta}\otimes\boldsymbol{\Delta}](t), \tag{6}$$

   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 equation (2). $\mathbb{T}(t)$ is shorthand for $\mathbb{T}(\boldsymbol{\Upsilon}(t))$, the t dependence being through the reference trajectory $\boldsymbol{\Upsilon}(t)$. The solution

of equation (6) is, formally, a time-ordered exponential,

$$[\boldsymbol{\Delta}\otimes\boldsymbol{\Delta}](t) = \exp_T\left(\int_0^t d\tau\, \mathbb{T}(\tau)\right)\cdot[\boldsymbol{\Delta}\otimes\boldsymbol{\Delta}](0)\,, \tag{7}$$

3. Average equation (7) over an ensemble of reference trajectories and then differentiate to form a new differential equation for $\langle\, \boldsymbol{\Delta}\otimes\boldsymbol{\Delta}\,\rangle(t)$,

$$\frac{d}{dt}\langle\, \boldsymbol{\Delta}\otimes\boldsymbol{\Delta}\,\rangle(t) = \mathbb{L}(t)\cdot\langle\, \boldsymbol{\Delta}\otimes\boldsymbol{\Delta}\,\rangle(t). \tag{8}$$

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 $|\boldsymbol{\Delta}(t)|^2 = Tr([\boldsymbol{\Delta}\otimes\boldsymbol{\Delta}](t))$, the Lyapunov exponent is,

$$\lambda = \tfrac{1}{2}\max \mathrm{Re}(\nu)\,. \tag{9}$$

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 $(+)$.

2.2 Perturbation theory

We shall apply a standard perturbation technique[15,8,1] to evaluate $\mathbb{L}(\infty)$ to second order (equation (10), below). In the dilute gas example (see Section 3, below), the zeroth and first order terms yield imaginary eigenvalues only (corresponding to oscillations). 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 equation (8) formally to second order in $\mathcal{T}_1$ gives an asymptotic evolution equation,[15,1]

$$\frac{d}{dt}\langle\, \boldsymbol{\Delta}\otimes\boldsymbol{\Delta}\,\rangle(t) \underset{t\to\infty}{=} \Big[\mathbb{T}_0 + \big\langle\, \mathbb{T}_1(t)\,\big\rangle + \int_0^\infty d\tau \big\langle\!\big\langle\, \mathbb{T}_1(t)\cdot e^{\tau\mathbb{T}_0}\cdot\mathbb{T}_1(t-\tau)\cdot e^{-\tau\mathbb{T}_0}\,\big\rangle\!\big\rangle\Big]\cdot\langle\, \boldsymbol{\Delta}\otimes\boldsymbol{\Delta}\,\rangle(t)\,. \quad (10)$$

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 R.M.S. magnitude of $\mathbb{T}_1(t)$, and τ_c is the characteristic autocorrelation decay time scale.

The form of $\mathbb{L}(\infty)$ in equation (10) allows us, already, to state the general rule that the Lyapunov exponent is a function of time integrals of correlation functions of the dynamical variables. The next section develops the theory in detail for the case of a dilute gas.

3 Application to a dilute gas or unmagnetized plasma

3.1 Perturbation from free particles

We consider a dilute gas or unmagnetized plasma with a hamiltonian of the form $H = \frac{1}{2}\boldsymbol{p}\cdot\boldsymbol{p} + V(\boldsymbol{q})$, where we have taken the particles to have unit mass. We partition the stability matrix, $\mathcal{T}$, of equation (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

$$\mathcal{T}_0 = \begin{pmatrix} 0 & 0 \\ \mathbf{1} & 0 \end{pmatrix}, \qquad \text{and,} \qquad \mathcal{T}_1(t) = \begin{pmatrix} 0 & -V_{\boldsymbol{qq}}(\boldsymbol{q}(t)) \\ 0 & 0 \end{pmatrix}. \tag{11}$$

The corresponding outer product operators are

$$\mathbb{T}_0 = \mathcal{T}_0 \otimes \mathbf{1} + \mathbf{1} \otimes \mathcal{T}_0, \qquad \text{and,} \qquad \mathbb{T}_1(t) = \mathcal{T}_1(t) \otimes \mathbf{1} + \mathbf{1} \otimes \mathcal{T}_1(t). \tag{12}$$

The first order term in equation (10) is simply,

$$\left\langle\, \mathbb{T}_1(t) \,\right\rangle = \mathbf{1} \otimes \left\langle\, \mathcal{T}_1(t) \,\right\rangle + \left\langle\, \mathcal{T}_1(t) \,\right\rangle \otimes \mathbf{1}. \tag{13}$$

We evaluate the exponential factor of the second order term by,

$$e^{\tau \mathbb{T}_0} = e^{\tau \mathcal{T}_0} \otimes e^{\tau \mathcal{T}_0}. \tag{14}$$

For ballistic motion, using equation (11), we have,

$$e^{\tau \mathcal{T}_0} = \begin{pmatrix} 1 & 0 \\ \tau & 1 \end{pmatrix}. \tag{15}$$

In order to understand better the explicit form of the integrand in the second order term of equation (10), 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:

$$\boldsymbol{\Delta} \otimes \boldsymbol{\Delta} \equiv \begin{pmatrix} \boldsymbol{\Delta}_p \otimes \boldsymbol{\Delta}_p \\ \boldsymbol{\Delta}_p \otimes \boldsymbol{\Delta}_q \\ \boldsymbol{\Delta}_q \otimes \boldsymbol{\Delta}_p \\ \boldsymbol{\Delta}_q \otimes \boldsymbol{\Delta}_q \end{pmatrix}. \tag{16}$$

In this representation the integrand in equation (10) becomes

$$\langle\!\langle\, \mathbb{T}_1(t)\cdot e^{\tau\mathbb{T}_0}\cdot \mathbb{T}_1(t-\tau)\cdot e^{-\tau\mathbb{T}_0}\,\rangle\!\rangle = \begin{pmatrix} -\tau^2\langle\!\langle\, \mathbb{v}_0\cdot\mathbb{v}_\tau+\mathbb{v}_0^{\mathsf{T}}\cdot\mathbb{v}_\tau^{\mathsf{T}}\,\rangle\!\rangle & \tau\langle\!\langle\, \mathbb{v}_0\cdot\mathbb{v}_\tau-\mathbb{v}_0\cdot\mathbb{v}_\tau^{\mathsf{T}}\,\rangle\!\rangle & \tau\langle\!\langle\, \mathbb{v}_0^{\mathsf{T}}\cdot\mathbb{v}_\tau^{\mathsf{T}}-\mathbb{v}_0^{\mathsf{T}}\cdot\mathbb{v}_\tau\,\rangle\!\rangle & \langle\!\langle\, \mathbb{v}_0\cdot\mathbb{v}_\tau^{\mathsf{T}}+\mathbb{v}_0^{\mathsf{T}}\cdot\mathbb{v}_\tau\,\rangle\!\rangle \\ \mathbf{0} & -\tau^2\langle\!\langle\, \mathbb{v}_0^{\mathsf{T}}\cdot\mathbb{v}_\tau^{\mathsf{T}}\,\rangle\!\rangle & -\tau^2\langle\!\langle\, \mathbb{v}_0^{\mathsf{T}}\cdot\mathbb{v}_\tau\,\rangle\!\rangle & \tau\langle\!\langle\, \mathbb{v}_0^{\mathsf{T}}\cdot\mathbb{v}_\tau+\mathbb{v}_0^{\mathsf{T}}\cdot\mathbb{v}_\tau^{\mathsf{T}}\,\rangle\!\rangle \\ \mathbf{0} & -\tau^2\langle\!\langle\, \mathbb{v}_0\cdot\mathbb{v}_\tau^{\mathsf{T}}\,\rangle\!\rangle & -\tau^2\langle\!\langle\, \mathbb{v}_0\cdot\mathbb{v}_\tau\,\rangle\!\rangle & \tau\langle\!\langle\, \mathbb{v}_0\cdot\mathbb{v}_\tau^{\mathsf{T}}+\mathbb{v}_0\cdot\mathbb{v}_\tau\,\rangle\!\rangle \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix}. \tag{17}$$

where $\mathbb{V}_\tau \equiv \mathbf{1}\otimes V_{\boldsymbol{qq}}(\boldsymbol{q}(t-\tau))$, and its transpose is,$\mathbb{V}_\tau^{\mathsf{T}} \equiv V_{\boldsymbol{qq}}(\boldsymbol{q}(t-\tau))\otimes\mathbf{1}$. The elements of the matrix in equation (17) have the structure of 1, τ, or τ^2, times a correlation function. The correlation functions are of two types,

$$\langle\!\langle\, \mathbb{V}_0\cdot\mathbb{V}_\tau\,\rangle\!\rangle = \mathbf{1}\otimes\langle\!\langle\, V_{\boldsymbol{qq}}(\boldsymbol{q}(t))\cdot V_{\boldsymbol{qq}}(\boldsymbol{q}(t-\tau))\,\rangle\!\rangle, \tag{18}$$

where the correlation itself has rank 2, and, rank 4 terms of the form,

$$\langle\!\langle\, \mathbb{V}_0^{\mathsf{T}}\cdot\mathbb{V}_\tau\,\rangle\!\rangle = \langle\!\langle\, V_{\boldsymbol{qq}}(\boldsymbol{q}(t))\otimes V_{\boldsymbol{qq}}(\boldsymbol{q}(t-\tau))\,\rangle\!\rangle. \tag{19}$$

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 the $\{\boldsymbol{p}(t),\boldsymbol{q}(t)\}$ which define the reference trajectories.

3.2 Equilibrium ensemble averaging

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 3-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 equations (13) and (17). 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, $\left\langle V_{\boldsymbol{q}_i \boldsymbol{q}_j}(0) \otimes V_{\boldsymbol{q}_k \boldsymbol{q}_l}(-\tau) \right\rangle$. 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 equation (13) the rotational isotropy simplifies each submatrix to

$$\left\langle V_{\boldsymbol{q}_i \boldsymbol{q}_j}(0) \right\rangle = \frac{1}{3} \left\langle Tr \left(V_{\boldsymbol{q}_i \boldsymbol{q}_j}(0) \right) \right\rangle \mathbf{1} \equiv \omega_{ij}^2 \mathbf{1}. \tag{20}$$

Similarly, each submatrix in equation (18) averages to

$$\begin{aligned} \langle\!\langle\, V_{\boldsymbol{q}\boldsymbol{q}}(\boldsymbol{q}(0)) \cdot V_{\boldsymbol{q}\boldsymbol{q}}(\boldsymbol{q}(-\tau)) \,\rangle\!\rangle_{ij} &= \frac{1}{3} \sum_{k=1}^{N} \left\langle\!\!\left\langle\, Tr \left(V_{\boldsymbol{q}_i \boldsymbol{q}_k}(\boldsymbol{q}(0)) \cdot V_{\boldsymbol{q}_k \boldsymbol{q}_j}(\boldsymbol{q}(-\tau)) \right) \right\rangle\!\!\right\rangle \mathbf{1} \\ &\equiv c_{ij}(\tau) \mathbf{1}. \end{aligned} \tag{21}$$

Rotational averaging the fourth rank subtensor (see Appendix A) of equation (19) gives

$$\langle\!\langle\, \mathbb{V}_0^{\mathsf{T}} \cdot \mathbb{V}_\tau \,\rangle\!\rangle_{ijkl} = a_{ijkl}(\tau) \mathbb{I} + b_{ijkl}(\tau) \mathbb{J}, \tag{22}$$

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,

$$\begin{aligned} a_{ijkl}(\tau) = \frac{1}{15} \Big[2 \left\langle\!\!\left\langle\, Tr \left(V_{\boldsymbol{q}_i \boldsymbol{q}_j}(\boldsymbol{q}(0)) \right) Tr \left(V_{\boldsymbol{q}_k \boldsymbol{q}_l}(\boldsymbol{q}(-\tau)) \right) \right\rangle\!\!\right\rangle - \\ \left\langle\!\!\left\langle\, Tr \left(V_{\boldsymbol{q}_i \boldsymbol{q}_j}(\boldsymbol{q}(0)) \cdot V_{\boldsymbol{q}_k \boldsymbol{q}_l}(\boldsymbol{q}(-\tau)) \right) \right\rangle\!\!\right\rangle \Big], \end{aligned} \tag{23}$$

and,

$$b_{ijkl}(\tau) = \frac{1}{30}\Big[- \Big\langle\Big\langle\, Tr\left(V_{\boldsymbol{q}_i\boldsymbol{q}_j}(\boldsymbol{q}(0))\right) Tr\left(V_{\boldsymbol{q}_k\boldsymbol{q}_l}(\boldsymbol{q}(-\tau))\right) \Big\rangle\Big\rangle + 3\Big\langle\Big\langle\, Tr\left(V_{\boldsymbol{q}_i\boldsymbol{q}_j}(\boldsymbol{q}(0)) \cdot V_{\boldsymbol{q}_k\boldsymbol{q}_l}(\boldsymbol{q}(-\tau))\right) \Big\rangle\Big\rangle \Big]. \quad (24)$$

3.3 Pairwise additive potential

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 averages from neighbors outside a small interaction volume, s. Since we are dealing with structureless particles, the potential energy between pair, a and b, has the form $\phi(|\boldsymbol{q}_a - \boldsymbol{q}_b|)$. The total potential energy is then

$$V = \frac{1}{2}\sum_{a=1}^{N}\sum_{b=1}^{N}\phi(|\boldsymbol{q}_a - \boldsymbol{q}_b|), \quad (25)$$

and,

$$V_{\boldsymbol{q}_i\boldsymbol{q}_j} = \delta_{ij}\sum_{b\neq i}^{N}\frac{\partial^2}{\partial\boldsymbol{q}_i^2}\phi(|\boldsymbol{q}_i - \boldsymbol{q}_b|) - (1-\delta_{ij})\frac{\partial^2}{\partial\boldsymbol{q}_i^2}\phi(|\boldsymbol{q}_i - \boldsymbol{q}_j|). \quad (26)$$

Under the dilute gas assumption we may neglect intrinsic 3 and 4 body correlations, that is, we may neglect correlations where the two particle pairs are not identical. For example, we shall take

$$\left\langle\!\!\left\langle \frac{\partial^2}{\partial\boldsymbol{q}_i^2}\phi(|\boldsymbol{q}_i(0) - \boldsymbol{q}_j(0)|) \cdot \frac{\partial^2}{\partial\boldsymbol{q}_k^2}\phi(|\boldsymbol{q}_k(-\tau) - \boldsymbol{q}_l(-\tau)|) \right\rangle\!\!\right\rangle = 0, \quad \{i,j\} \neq \{k,l\}. \quad (27)$$

Each particle pair contributes $O\left(\frac{s\,n}{N}\right)$ to the average, where n is the mean particle density. Discarding terms $O\left(\frac{1}{N}\right)$, leaves just ω_{ii}^2, $c_{ii}(\tau)$, $a_{iiii}(\tau)$ and $b_{iiii}(\tau)$. The same assumptions also give

$$c_{ii}(\tau) = 2\left[a_{iiii}(\tau) + 4b_{iiii}(\tau)\right]. \tag{28}$$

With these simplifications, the differential equation, (10), decouples by particle.

3.4 Eigenvalues of separation evolution

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 eigen-directions of the operator $\mathbb{J}$. The only eigen-direction which can contribute to $\left\langle\, |\boldsymbol{\Delta}|^2 \,\right\rangle$ has eigenvalue[1], $J = 4$ (see Appendix B). 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,

$$c_m \equiv \int_0^\infty d\tau\, \tau^m c_{ii}(\tau); \qquad m = 0,\, 1,\, \text{or}\, 2, \tag{29}$$

the resulting matrix whose eigenvalues we seek is

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -\omega_{ii}^2 & -\omega_{ii}^2 & 0 \\ 0 & 0 & 0 & -\omega_{ii}^2 \\ 0 & 0 & 0 & -\omega_{ii}^2 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} -2c_2 & \frac{1}{2}c_1 & \frac{1}{2}c_1 & c_0 \\ 0 & -c_2 & -\frac{1}{2}c_2 & \frac{3}{2}c_1 \\ 0 & -\frac{1}{2}c_2 & -c_2 & \frac{3}{2}c_1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{30}$$

The eigenvalues, ν, of matrix (30) are discussed in Appendix C. The Lyapunov exponent is given by, $\lambda = \frac{1}{2}\max \mathrm{Re}(\nu)$. 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 auto-correlation time is short, then c_0 dominates terms with c_1 or c_2 in the secular equation. If we take this to be so then there is indeed a solution with positive $\mathrm{Re}(\nu)$, namely, $\nu = \left[2c_0\right]^{1/3}$. Hence the Lyapunov exponent for a dilute gas (or unmagnetized plasma) in equilibrium is given by,

$$\lambda = \left[\frac{c_0}{4}\right]^{1/3} = \left[\frac{1}{6}\int_0^\infty d\tau \left\langle\!\!\left\langle\, Tr(\, V_{\boldsymbol{q}_i \boldsymbol{q}_i}(0) \cdot V_{\boldsymbol{q}_i \boldsymbol{q}_i}(-\tau)\,)\,\right\rangle\!\!\right\rangle\right]^{1/3} \tag{31}$$

3.5 Lyapunov exponent and fluctuations

Equation (31) shows the equilibrium Lyapunov exponent to be proportional to the cube root of the integral of an auto-correlation function of the fluctuations of a dynamical variable. The fluctuation-dissipation theorem[14,16] relates linear response functions to corresponding correlation integrals. The correlation in equation (31) 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 self-diffusion coefficient is proportional to the time integral a particle's velocity autocorrelation,

$$D = \frac{1}{3}\int_0^\infty d\tau \,\langle\!\langle\, \boldsymbol{v}(0) \cdot \boldsymbol{v}(\tau)\,\rangle\!\rangle. \tag{32}$$

(Note that this quantity is distinct from the spatial diffusion coefficient which becomes large in the collisionless limit while self-diffusion does not). This leads us to suggest that the Lyapunov exponent is proportional to the cube root of the diffusion coefficient,

$$\frac{\lambda}{\omega_p} \propto \left[\frac{D}{\omega_p a_i^2}\right]^{1/3}, \tag{33}$$

where ω_p is a characteristic interaction frequency and a_i is a characteristic inter-particle distance.

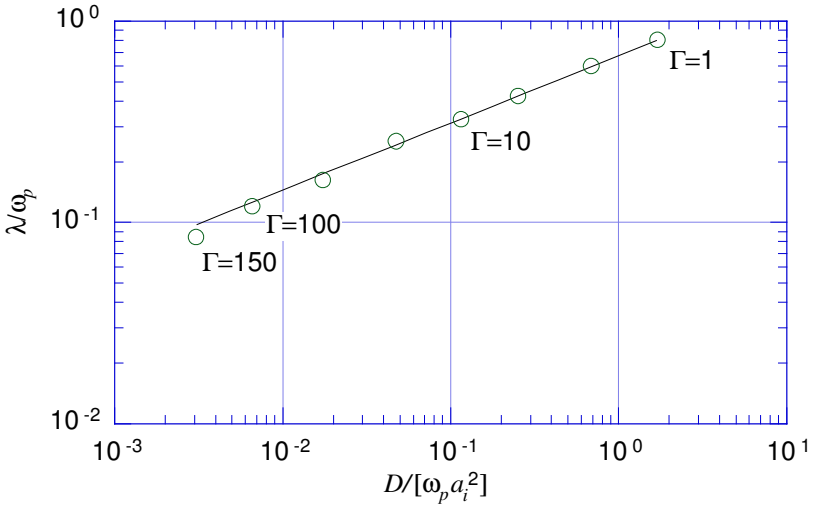

Figure 2: Lyapunov exponent versus diffusion coefficient for plasma parameter, Γ, values between 1 and 150. The data were computed for a one component plasma by Nishihara et al.[2–4] The line is $\lambda = a\, D^{1/3}$—the law suggested by the theory.

In numerical simulations, Nishihara et al.[2–4] measured both the Lyapunov exponent and the self-diffusion coefficient for the ions in a one component plasma. The results, plotted in Figure 2, clearly show a one third power dependence of Lyapunov exponent on diffusion coefficient over nearly three decades of diffu-

sion data. This one third power relationship with a transport coefficient is a consequence of the dilute gas Lyapunov exponent theory.

4 One component plasma example

We now apply the theory to a one component plasma. The plasma will comprise protons of mass, m_p, and charge, q_e, in a uniform neutralizing background. The interaction is via the Coulomb potential, $\phi(\boldsymbol{r}) = \frac{q_e^2}{r}$. The rotational average of the second derivative of this potential is identically zero because $\nabla^2 \frac{1}{r} = 0$. The Coulomb force gives rise to long range correlations amongst the ions, leading to Debye screening. With care, one can evaluate equation (31) using the Coulomb potential and an ensemble with a radial distribution function, $g(r_{ij}) = n_p - [k_D^2/4\pi]\exp(-k_D r_{ij})/r_{ij}$. ($n_p$ is the ion number density and k_D is the inverse Debye screening length). However, in the exposition which follows, we shall get the same answer by absorbing the pair correlation function into an effective Debye-screened potential,

$$\phi(\boldsymbol{r}) = \frac{q_e^2}{r} e^{-k_D r}, \tag{34}$$

and using an uncorrelated ensemble. For convenience, we shall use units with $m_p = 1$ and then restore mass units at the end.

The potential energy of the ion system is given by,

$$V = \frac{1}{2}\sum_{a=1}^{N}\sum_{b=1}^{N}\phi(|\boldsymbol{q}_a - \boldsymbol{q}_b|). \tag{35}$$

Since the plasma is supposed dilute we shall treat the interaction between two ions as ballistic,

$$\boldsymbol{q}_i(-\tau) = \boldsymbol{q}_i(0) - \boldsymbol{p}_i\tau. \tag{36}$$

With this approximation it is most convenient to use a Fourier representation of the second derivative of the potential energy,

$$V_{\boldsymbol{q}_i\boldsymbol{q}_i}(-\tau) = -\sum_{b\neq i}\int d^3\boldsymbol{k}\,\boldsymbol{k}\boldsymbol{k}\,\tilde{\phi}(\boldsymbol{k})\,e^{i\boldsymbol{k}\cdot[\boldsymbol{q}_i-\boldsymbol{q}_b]}\,e^{-i\boldsymbol{k}\cdot[\boldsymbol{p}_i-\boldsymbol{p}_b]\tau}, \tag{37}$$

where the Fourier transform of $\phi(\boldsymbol{r})$ is

$$\tilde{\phi}(\boldsymbol{k}) = \frac{4\pi\,q_e^2}{[2\pi]^3}\frac{1}{k^2+k_D^2}, \tag{38}$$

and we have written $\boldsymbol{q}_i \equiv \boldsymbol{q}_i(0)$.

In averaging the cross-correlation, $c_{ii}(\tau) \equiv \frac{2}{3}\langle\!\langle\, Tr(V_{\boldsymbol{q}_i\boldsymbol{q}_i}(0)\cdot V_{\boldsymbol{q}_i\boldsymbol{q}_i}(-\tau))\,\rangle\!\rangle$, we shall use an ensemble distribution uniform in space and maxwellian in momentum. We shall neglect correlation distribution (beyond our effective potential) because the residual effects of this are of a higher order than the term itself. The multi-particle distribution function thus factors into a product of one-particle distributions,

$$f_1(\boldsymbol{q}_i,\boldsymbol{p}_i) = \frac{n_p}{N}[2\pi T_p]^{-3/2}\exp\left(-\frac{p_i^2}{2T_p}\right), \tag{39}$$

where n_p is the ion density, T_p is the ion temperature in energy units. The cross-correlation contains a double sum over ions different from i arising from the double application of equation (37). Where the two ions are different, the spatial integral of the ensemble average on the complex exponential factor yields,

$$\frac{1}{[2\pi]^3}\int d^3\boldsymbol{q}_b\,e^{i\boldsymbol{k}\cdot\boldsymbol{q}_b} = \delta^3(\boldsymbol{k}). \tag{40}$$

The $\delta^3(\boldsymbol{k})$ is multiplied by $\boldsymbol{k}$ so the result is zero. This is consistent with the assumption, used in the dilute gas theory, that disjoint pairs of particles are

uncorrelated. Hence only the $N-1$ diagonal terms in the double sum contribute to the correlation, $c_{ii}(\tau)$. They evaluate identically to give,

$$c_{ii}(\tau) = \frac{2}{3}[N-1]\frac{[4\pi]^2 q_e^4}{[2\pi]^6}\left[\frac{n_p}{N}\right]^2 [2\pi T_p]^{-3}\int d^3\boldsymbol{p}_i d^3\boldsymbol{p}_b \exp\left(-\frac{p_i^2+p_b^2}{2T_p}\right) \quad \times$$
$$\int d^3\boldsymbol{q}_i d^3\boldsymbol{q}_b \int d^3\boldsymbol{k}_0 \int d^3\boldsymbol{k}_\tau \frac{[\boldsymbol{k}_0\cdot\boldsymbol{k}_\tau]^2}{[k_0^2+k_D^2][k_\tau^2+k_D^2]} e^{i[\boldsymbol{k}_0+\boldsymbol{k}_\tau]\cdot[\boldsymbol{q}_i-\boldsymbol{q}_b]} e^{-i\boldsymbol{k}_\tau\cdot[\boldsymbol{p}_i-\boldsymbol{p}_b]\tau}. \quad (41)$$

Changing the order of integration to perform the real space ($\boldsymbol{q}_i$ and $\boldsymbol{q}_b$) integrals first yields two factors of $\delta^3(\boldsymbol{k}_0+\boldsymbol{k}_\tau)$. Taking into account the finite real volume we should interpret the space integrals as,

$$\int d^3\boldsymbol{q}_i d^3\boldsymbol{q}_b\, e^{i[\boldsymbol{k}_0+\boldsymbol{k}_\tau]\cdot[\boldsymbol{q}_i-\boldsymbol{q}_b]} = [2\pi]^3\frac{N}{n_p}\delta^3(\boldsymbol{k}_0+\boldsymbol{k}_\tau). \quad (42)$$

Performing the $\boldsymbol{k}_0$ triple integral then sets $\boldsymbol{k}\equiv\boldsymbol{k}_\tau=-\boldsymbol{k}_0$. Using these results in equation (41), and neglecting 1 compared to N gives,

$$c_{ii}(\tau) = \frac{\frac{2}{3}[4\pi]^2 q_e^4\, n_p}{[2\pi]^3[2\pi T_p]^3}\int d^3\boldsymbol{p}_i d^3\boldsymbol{p}_b \exp\left(-\frac{p_i^2+p_b^2}{2T_p}\right)\int d^3\boldsymbol{k}\,\frac{k^4}{[k^2+k_D^2]^2} e^{-i\boldsymbol{k}\cdot[\boldsymbol{p}_i-\boldsymbol{p}_b]\tau}. \quad (43)$$

Next we perform the momentum integrals,

$$c_{ii}(\tau) = \frac{2}{3}\frac{[4\pi]^2 q_e^4\, n_p}{[2\pi]^3}\int d^3\boldsymbol{k}\,\frac{k^4}{[k^2+k_D^2]^2}\exp(-T_p\,k^2\,\tau^2), \quad (44)$$

and the angular part of the $\boldsymbol{k}$ integral to get,

$$c_{ii}(\tau) = \frac{16}{3}q_e^4\, n_p\int dk\,\frac{k^6}{[k^2+k_D^2]^2}\exp(-T_p\,k^2\,\tau^2). \quad (45)$$

The cross-correlation in equation (31) is the time integral of $c_{ii}(\tau)$. Performing this integral yields,

$$c_0 = \frac{16}{3} q_e^4 n_p \int dk \, \frac{k^6}{[k^2 + k_D^2]^2} \, \frac{\pi^{1/2} m_p^{1/2}}{2 T_p^{1/2} k}, \tag{46}$$

where we have also restored mass units by writing $\frac{T_p}{m_p}$ everywhere T_p occurred. This last integral diverges as $k \to \infty$. The ions almost never have encounters at very short distances, however, (and when they do the ballistic encounter approximation fails severely). We shall, therefore, truncate the integral at an upper limit of $k_{\max}$. It is also convenient to write the integral in dimensionless form using a scaled variable, $x = k/k_D$, and to rewrite the dimensioned coefficients in terms of the plasma frequency, given by $\omega_p^2 = \frac{4\pi n_p q_e^2}{m_p} = k_D^2 \frac{T_p}{m_p}$, and the dimensionless plasma parameter, $\Gamma = \left[\frac{4\pi}{3} n_p\right]^{1/3} \frac{q_e^2}{T_p} \equiv \frac{q_e^2}{a_i T_p}$. The result is,

$$c_0 = m_p^2 \omega_p^3 \, \frac{2}{3^{1/2} \pi^{1/2}} \Gamma^{3/2} \int_0^{x_{max}} dx \, \frac{x^5}{[x^2 + 1]^2}. \tag{47}$$

Evaluating the integral and substituting into equation (31) gives the Lyapunov exponent,

$$\lambda = \left[\frac{c_0}{4 m_p^2}\right]^{1/3} = \omega_p \left[\frac{2}{3^{1/2} \pi^{1/2}} \Gamma^{3/2}\right]^{1/3} \left[-\frac{1}{2} \frac{x_{max}^4}{1 + x_{max}^2} + x_{max}^2 - \ln\left(1 + x_{max}^2\right)\right]^{1/3}. \tag{48}$$

The choice of $k_{\max}$ (and hence x_{max}) must be determined by physical considerations. Variations in the plasma with a half-wavelength smaller than the order of the inter-ion spacing, a_i, are not meaningful. We therefore suggest a cutoff, $k_{\max} = \pi / a_i$, that is,

$$x_{max} \equiv \frac{k_{\max}}{k_D} = \frac{\pi}{3^{1/2} \Gamma^{1/2}}. \tag{49}$$

We shall now consider some limiting plasma cases.

4.1 Dilute plasma limit

In the limit of a hot or sparse plasma whose plasma parameter, $\Gamma \ll 1$, we have $x_{max} \gg 1$, and the last square bracket in equation (48) goes asymptotically as $x_{max}^2/2$, giving us a plasma parameter dependence of

$$\frac{\lambda}{\omega_p} \propto \Gamma^{1/6} \qquad \text{when} \quad \Gamma \ll 1. \tag{50}$$

4.2 Liquid plasma limit

In the cold dense liquid plasma limit, when $\Gamma \gtrsim 1$, we have $x_{max} < 1$, and the last square bracket in equation (48) goes asymptotically as $x_{max}^6/6$, giving us a plasma parameter dependence of

$$\frac{\lambda}{\omega_p} \propto \Gamma^{-1/2} \qquad \text{when} \quad \Gamma \gg 1. \tag{51}$$

5 Comparison with numerical simulations

Nishihara et al.[3,4] have used the SCOPE particle-particle particle-mesh program to simulate a one component plasma in equilibrium for a range of values of the plasma parameter, Γ. The program was adapted to calculate the Lyapunov exponent by following the evolution of two initial conditions differing slightly from one another. For $170 > \Gamma \gtrsim 1$ their results are consistent with the $\Gamma^{-1/2}$ law derived above. For $\Gamma \lesssim 1$ they find the Lyapunov exponent to be nearly constant.

6 Discussion and conclusions

We have shown that the Lyapunov exponent of a dilute gas in equilibrium is proportional to the cube root of a fluctuation correlation function. One of the surprises of Figure 2 is that this cube root law holds even for fairly dense plasmas. When estimating the eigenvalues of the matrix (30), we assumed that we could neglect terms with c_1 and c_2 compared to c_0. In the dense regime, these terms bear a simple relation to one another. As a result the secular equation in Appendix C may be written simply in terms of c_0. The eigenvalue remains proportional to $c_0^{1/3}$ but with a different constant numerical coefficient.

Other workers have found one third power rules between a diffusion coefficient and exponential path separation in different contexts. Seki et al.[17] used a Langevin equation to explore diffusion in turbulent media. For intermediate times, they found, adjacent fluid elements separate exponentially at a rate proportional to the one third power of the long term diffusion constant. In Dupree's[18] theory of plasma turbulence, a mode's exponential growth rate is proportional to the one third power of the velocity space diffusion constant which is proportional to the turbulent fluctuations.

The theory developed in this paper might find application in other many body systems, such as the cosmological scattering of photons by gravitational lensing, where Fukushige et al.[19] have noted an exponential path divergence for adjacent light rays undergoing multiple scattering.

This theory might also be applied to study the diffusion of trace elements due to environmental fluctuations.

This paper developed the ab initio Lyapunov exponent theory for the example

of a dilute gas near equilibrium. A future paper will develop an example for lattice vibrations of an anharmonic crystal.

Our theory establishes firmly the connection between the many body Lyapunov exponent and fluctuations. We believe that the Lyapunov expansion rate should be regarded as a system parameter. Since it is readily definable almost anywhere in phase space, it can provide a link between states near to and far from equilibrium.

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Appendix A

Rotational averaging of rank four tensors

This appendix considers the rotational averaging of a fourth rank tensor with outer product form, $\mathcal{A}\otimes\mathcal{B}$.

In cartesian components, the rotationally averaged outer product tensor must have the form of an isotropic fourth rank tensor,

$$\langle \mathcal{A}\otimes\mathcal{B} \rangle_{\alpha\beta\gamma\delta} = a\,\delta_{\alpha\beta}\,\delta_{\gamma\delta} + b\,\delta_{\alpha\gamma}\,\delta_{\beta\delta} + c\,\delta_{\alpha\delta}\,\delta_{\beta\gamma}. \qquad (A\text{–}1)$$

To evaluate the coefficients a, b, and c, we can perform tracing (contracting) over pairs of indices, since the trace operation commutes with a rotational average:

$$\langle\, Tr(\mathcal{A})Tr(\mathcal{B})\,\rangle = 9a + 3b + 3c; \qquad \alpha \text{ with } \beta, \text{ and } \gamma \text{ with } \delta. \qquad (A\text{–}2)$$

$$\left\langle\, Tr(\mathcal{A}^{\mathsf{T}}\cdot\mathcal{B})\,\right\rangle = 3a + 9b + 3c; \qquad \alpha \text{ with } \gamma, \text{ and } \beta \text{ with } \delta. \qquad (A\text{–}3)$$

$$\langle\, Tr(\mathcal{A}\cdot\mathcal{B})\,\rangle = 3a + 3b + 9c; \qquad \alpha \text{ with } \delta, \text{ and } \beta \text{ with } \gamma. \qquad (A\text{–}4)$$

Solving for the coefficients gives,

$$a = \frac{1}{30}\left[4\langle\, Tr(\mathcal{A})Tr(\mathcal{B})\,\rangle - \left\langle\, Tr(\mathcal{A}^{\mathsf{T}}\cdot\mathcal{B})\,\right\rangle - \langle\, Tr(\mathcal{A}\cdot\mathcal{B})\,\rangle\right], \qquad (A\text{–}5)$$

$$b = \frac{1}{30}\left[4\left\langle\, Tr(\mathcal{A}^{\mathsf{T}}\cdot\mathcal{B})\,\right\rangle - \langle\, Tr(\mathcal{A}\cdot\mathcal{B})\,\rangle - \langle\, Tr(\mathcal{A})Tr(\mathcal{B})\,\rangle\right], \qquad (A\text{–}6)$$

$$c = \frac{1}{30}\left[4\langle\, Tr(\mathcal{A}\cdot\mathcal{B})\,\rangle - \left\langle\, Tr(\mathcal{A}^{\mathsf{T}}\cdot\mathcal{B})\,\right\rangle - \langle\, Tr(\mathcal{A})Tr(\mathcal{B})\,\rangle\right]. \qquad (A\text{–}7)$$

If either $\mathcal{A}$ or $\mathcal{B}$ is symmetric then the solution further simplifies to

$$\langle \mathcal{A}\otimes\mathcal{B} \rangle = a\,\mathbb{I} + b\,\mathbb{J}, \qquad (A\text{–}8)$$

where,

$$\mathbb{J}_{\alpha\beta\gamma\delta} = \delta_{\alpha\gamma}\,\delta_{\beta\delta} + \delta_{\alpha\delta}\,\delta_{\beta\gamma}, \qquad \text{and,} \qquad \mathbb{I} \equiv \mathbf{1}\otimes\mathbf{1}, \qquad (A\text{–}9)$$

and,

$$a = \frac{1}{15}\left[2\,\langle\, Tr(\mathcal{A})Tr(\mathcal{B})\,\rangle - \langle\, Tr(\mathcal{A}\cdot\mathcal{B})\,\rangle\right], \qquad (A\text{–}10)$$

and,

$$b = \frac{1}{30}\left[-\,\langle\, Tr(\mathcal{A})Tr(\mathcal{B})\,\rangle + 3\,\langle\, Tr(\mathcal{A}\cdot\mathcal{B})\,\rangle\right]. \qquad (A\text{–}11)$$

Appendix B

Eigenvalues of non outer product rank 4 operator

The isotropic fourth rank tensor $\mathbb{J}$, defined in Appendix A,

$$\mathbb{J}_{\alpha\gamma\beta\delta} = \delta_{\alpha\beta}\,\delta_{\gamma\delta} + \delta_{\alpha\delta}\,\delta_{\beta\gamma}, \tag{B–1}$$

does not have outer product form with respect to operations on a second rank tensor, $\mathcal{X}_{\gamma\delta}$. We wish to find its eigenvalues, J, and eigentensors, $\mathcal{X}$, solutions of the equation,

$$\mathbb{J}_{\alpha\gamma\beta\delta}\mathcal{X}_{\gamma\delta} = J\,\mathcal{X}_{\alpha\beta}, \tag{B–2}$$

where a repeated pair of indices implies contraction over that pair.

By inspection we can identify the eigentensor with eigenvalue $J = 4$,

$$\begin{aligned} \mathcal{X}_{\gamma\delta} &= \delta_{\gamma\delta} \\ &\equiv [\hat{\boldsymbol{x}}\otimes\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}\otimes\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}\otimes\hat{\boldsymbol{z}}]_{\gamma\delta}\,, \end{aligned} \tag{B–3}$$

where $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{y}}$, and $\hat{\boldsymbol{z}}$ are the cartesian unit vectors. In the coordinate system where $\hat{\boldsymbol{x}}_\alpha = \delta_{1\alpha}$, $\hat{\boldsymbol{y}}_\alpha = \delta_{2\alpha}$, and, $\hat{\boldsymbol{z}}_\alpha = \delta_{3\alpha}$, we can express the five eigentensors with eigenvalue, $J = 1$, as

$$[\hat{\boldsymbol{x}}\otimes\hat{\boldsymbol{y}} + \hat{\boldsymbol{y}}\otimes\hat{\boldsymbol{x}}], \qquad [\hat{\boldsymbol{y}}\otimes\hat{\boldsymbol{z}} + \hat{\boldsymbol{z}}\otimes\hat{\boldsymbol{y}}], \qquad [\hat{\boldsymbol{z}}\otimes\hat{\boldsymbol{x}} + \hat{\boldsymbol{x}}\otimes\hat{\boldsymbol{z}}],$$

and, (B–4)

$$[\hat{\boldsymbol{x}}\otimes\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}\otimes\hat{\boldsymbol{y}}], \quad \text{and,} \quad [\hat{\boldsymbol{y}}\otimes\hat{\boldsymbol{y}} - \hat{\boldsymbol{z}}\otimes\hat{\boldsymbol{z}}].$$

There are three eigentensors with eigenvalue, $J = -1$,

$$[\hat{\boldsymbol{x}}\otimes\hat{\boldsymbol{y}} - \hat{\boldsymbol{y}}\otimes\hat{\boldsymbol{x}}], \qquad [\hat{\boldsymbol{y}}\otimes\hat{\boldsymbol{z}} - \hat{\boldsymbol{z}}\otimes\hat{\boldsymbol{y}}], \quad \text{and,} \qquad [\hat{\boldsymbol{z}}\otimes\hat{\boldsymbol{x}} - \hat{\boldsymbol{x}}\otimes\hat{\boldsymbol{z}}]. \tag{B–5}$$

Only the $J = 4$ eigentensor in (B–3) has a nonzero trace which can contribute to the mean square length, $\left\langle\, |\boldsymbol{\Delta}|^2 \,\right\rangle$.

Appendix C

Eigenvalues of dilute gas Lyapunov matrix

The 4×4 matrix in (30) is the asymptotic operator which gives the Lyapunov expansion. The expansion will be dominated by the eigenvalue, ν, with the largest real part. Since the operator is part of the evolution equation for the square of the phase-space separation, the Lyapunov exponent is half this eigenvalue,

$$\lambda = \frac{1}{2} \max \mathrm{Re}(\nu). \qquad (C\text{–}1)$$

The secular equation for the eigenvalues of (30) is

$$\det \begin{vmatrix} -\nu - 2c_2 & \frac{1}{2}c_1 - \omega_{ii}^2 & \frac{1}{2}c_1 - \omega_{ii}^2 & c_0 \\ 1 & -\nu - c_2 & -\frac{1}{2}c_2 & \frac{3}{2}c_1 - \omega_{ii}^2 \\ 1 & -\frac{1}{2}c_2 & -\nu - c_2 & \frac{3}{2}c_1 - \omega_{ii}^2 \\ 0 & 1 & 1 & -\nu \end{vmatrix} = 0\,, \qquad (C\text{–}2)$$

which expands to

$$\left[\nu + \tfrac{1}{2}c_2\right] \left[\nu^3 + \tfrac{7}{2}c_2\,\nu^2 + \left[3c_2^2 - 4\left[c_1 - \omega_{ii}^2\right]\right]\nu - 6c_1c_2 - 2c_0\right] = 0. \qquad (C\text{–}3)$$

It is instructive to analyze the solutions of equation (C–3) for various ranges of the parameters,

$$\nu = \begin{cases} 0,\ \left[2c_0\right]^{1/3},\ \text{or}\ \left[2c_0\right]^{1/3} e^{\pm 2i\pi/3}, & \text{with (a)} \quad c_2 = c_1 = \omega_{ii}^2 = 0; \\ 0,\ 0,\ \text{or}\ \pm 2\left[c_1 - \omega_{ii}^2\right]^{1/2}, & \text{with (b)} \quad c_2 = c_0 = 0; \\ 0,\ -\frac{1}{2}c_2,\ -\frac{3}{2}c_2,\ \text{or}\ -2c_2, & \text{with (c)} \quad c_0 = c_1 = \omega_{ii}^2 = 0. \end{cases} \qquad (C\text{–}4)$$

In case (c), $\nu \leq 0$, so it cannot produce Lyapunov expansion. Case (b) can have a positive ν if $c_1 > \omega_{ii}^2$ (otherwise the nonzero eigenvalues are imaginary). Case (a) has one unequivocally positive solution, namely $\nu = \left[2c_0\right]^{1/3}$.

To consider the relative magnitudes of the parameters we introduce the correlation time, τ_c, which we wish to treat as a small parameter in the same sense that the Kubo number, $\alpha\,\tau_c$, was a small parameter in Section 2.2 and reference[15]. Then we may expect the following,

$$c_1 \simeq \tau_c\, c_0, \qquad \text{and,} \qquad c_2 \simeq \frac{1}{2}\tau_c^2 c_0\,. \tag{C–5}$$

Suppose that

$$\nu = \nu_0 + \beta\,\nu_1 + \beta^2\,\nu_2 + \cdots, \tag{C–6}$$

where β is used to keep track of perturbation order and we shall set it to 1 at the end. In equation (C–3) we shall rewrite c_2 as $\beta^2\,c_2$, and c_1 as $\beta\,c_1$. We shall also take $\omega_{ii}^2 = O(\beta)$. Equating coefficients of powers of β gives,

$$\nu_0^3 - 2\,c_0 = 0, \tag{C–7}$$

$$3\nu_0^2\,\nu_1 - 4\left[c_1 - \omega_{ii}^2\right]\nu_0 = 0, \tag{C–8}$$

etc. which give us,

$$\nu_0 = \left[2\,c_0\right]^{1/3}, \qquad \text{and,} \qquad \nu_1 = \frac{4}{3\left[2\,c_0\right]^{1/3}}\left[c_1 - \omega_{ii}^2\right]. \tag{C–9}$$

To leading order, then,

$$\lambda = \frac{1}{2}\left[2\,c_0\right]^{1/3}.$$

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