Comment on “Lyapunov Exponent of a Many Body System and Its Transport Coefficients”

In a recent Letter, Barnett, Tajima, Nishihara, Ueshima, and Furukawa [1] obtained a theoretical expression for the maximum Lyapunov exponent $\lambda_1$ of a dilute gas. They conclude that $\lambda_1$ is proportional to the cube root of the self-diffusion coefficient $D$, independent of the range of the interaction potential. They validate their conjecture with numerical data for a dense one-component plasma, a system with long-range forces. We claim that their result is highly nongeneric. We show in the following that it does not apply to a gas of hard spheres, neither in the dilute nor in the dense phase.

Systems of hard spheres have properties similar to real fluids and solids and provide a reference for successful perturbation theories [2]. Simulations with this model were able to uncover fundamental aspects of collective particle dynamics such as recollisions and the “cage” effect [2]. Hard-sphere systems are also paradigms for chaotic and ergodic properties of many body systems with short-range interactions, and were shown to have a positive Kolmogorov-Sinai entropy [3,4].

For dilute gases, Krylov [5] provided an analytical estimate for the maximum Lyapunov exponent,

$$\lambda_1 = -(32\pi K / 3mN)^{1/2} \sigma^2 n \log(\pi \sigma^3 n / \sqrt{2}), \quad (1)$$

where $K$ is the kinetic energy, $N$ is the number of particles, $m$ is the particle mass, $n$ is the number density, and $\sigma$ is the hard-sphere diameter. This expression has been verified numerically (apart from a factor $\sim 2.8$ [4]), and has been extended to larger densities [6].

The diffusion coefficient for dilute hard-sphere gases is well approximated by the Enskog expression [7],

$$D_E = (3\pi K / 2mN)^{1/2} \frac{1}{n\pi\sigma^3} \left[ 1 + \frac{5n\pi\sigma^3}{12} \right]^{-1}. \quad (2)$$

A comparison of Eqs. (1) and (2) reveals that, in the dilute gas limit, the proposed relation $\lambda_1 \propto D^{1/3}$ of Barnett et al. cannot be satisfied. Moreover, we combine in Fig. 1 recent simulation results for $D$ and $\lambda_1$, which were obtained for a system of 500 hard spheres over the full range of fluid densities ($0.0001 < n\sigma^3 < 0.89$). Reduced units are used for which $\sigma$, $m$, and the kinetic energy per particle $K/N$ are all unity. One observes that these data are not consistent with the proposed $D^{1/3}$ dependence (solid line), neither for low densities nor for large.

We conclude that the conjecture by Barnett et al. does not apply to many body systems with short-range interactions. But even its applicability for long-range interactions is doubtful. A one-dimensional gravitational system with finite $N$ exhibits a positive $\lambda_1$ [8], whereas this clustering and confining system does not show diffusion. We also note that, while the theoretical expression (26) in Ref. [1] has been obtained for a dilute gas, the data in Fig. 1 of Ref. [1] are for a dense plasma with a Coulomb coupling constant $\Gamma$ ranging from 1 to 150. As reported by the same authors [9], for $\Gamma > 1$ the plasma behaves as a liquid and not as a gas. The dilute gas limit is recovered only for $\Gamma \ll 1$ [9].

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A. Torcini,¹ Ch. Dellago,² and H. A. Posch³
¹Dipartimento di Energetica
INFM, Unità di Firenze
I-50139 Firenze, Italy
²Department of Chemistry
University of California
Berkeley, California 94720
³Institut für Experimentalphysik
Universität Wien
Boltzmanngasse 5
A-1090 Wien, Austria

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