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 λ_1 of a dilute gas. They conclude that λ_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 the 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 σ is the hard-sphere diameter. This expression has been verified numerically (apart from a factor ~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],

$$D_E = (3\pi K/32mN)^{1/2} \frac{1}{n\pi\sigma^2} \left[1 + \frac{5n\pi\sigma^3}{12} \right]^{-1}.$$
 (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 λ_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 σ , 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 λ_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



FIG. 1. Simulation results $\lambda_1 = \lambda_1(D)$ (crosses) for a gas of hard spheres. The solid line refers to the expression $\lambda_1 \propto D^{1/3}$ suggested in Ref. [1].

data in Fig. 1 of Ref. [1] are for a dense plasma with a Coulomb coupling constant Γ 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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- D. M. Barnett, T. Tajima, K. Nishihara, Y. Ueshima, and H. Furukawa, Phys. Rev. Lett. 76, 1812 (1996).
- [2] J.P. Boon and S. Yip, *Molecular Hydrodynamics* (McGraw-Hill, New York, 1980).
- [3] H. van Beijeren, J.R. Dorfman, H.A. Posch, and Ch. Dellago, Phys. Rev. E 56, 5272 (1997).
- [4] Ch. Dellago and H. A. Posch, Physica (Amsterdam) 240A, 68 (1997).
- [5] N.S. Krylov, Works on the Foundations of Statistical Mechanics (Princeton University Press, Princeton, NJ, 1979).
- [6] R. van Zon, H. van Beijeren, and Ch. Dellago, Phys. Rev. Lett. 80, 2035 (1998).
- [7] S. Chapman and T. G. Cowling, *The Mathematical Theory* of Non-Uniform Gases (Cambridge University Press, Cambridge, England, 1970).
- [8] Lj. Milanović, H. A. Posch, and W. Thirring, Phys. Rev. E 57, 2763 (1998).
- [9] Y. Ueshima et al., Phys. Rev. E 55, 3439 (1997).

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