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Numerical Evidence for the Low-Mass Behavior of the One-Dimensional Rayleigh Gas with Local Interaction

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Numerical investigations, supported by partial rigorous results suggest that the motion of a tagged particle of mass M on the line $\mathbb{R}^1$ colliding with a free gas of particles of mass m in equilibrium is diffusive. It was conjectured that the diffusion constant $D(M)$, for small mass $M \to 0$, should approach $D(m)$. (In dimension 1 this is a kind of "continuity hypothesis.") Previous results of computer simulations are inconclusive. We report on some new computer results, which show clearly that there is no continuity, and the limit of $D(M)$ as $M \to 0$ is smaller than $D(m)$. We compare with the corresponding results for a similar two-dimensional model, to which the "continuity argument" cannot be applied.

KEY WORDS: Rayleigh gas; Brownian limit; diffusion.

1. INTRODUCTION

The Rayleigh gas, i.e., the motion of a singled-out particle in a gas, is the standard model for investigating the appearance of Brownian motion in deterministic mechanical systems. Due to the well known difficulties in controlling the evolution of infinitely many interacting particles, rigorous investigations are restricted to the case when the interaction is "localized" around the Rayleigh particle ("R.p." for short), i.e., the particles of the gas interact only with the R.p., by elastic collisions or by a short-range interaction. The main idea underlying possible rigorous proofs is that, if the effect of the interaction on the distribution of the surrounding gas can

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be in some sense neglected, the displacement of the R.p. can be approximately considered as a sum of increments due to independent "collisions," so that, in the appropriate scaling, it will tend to the Brownian limit.

A few years ago several authors[1–4] devoted their attention to the Rayleigh gas, and some rigorous results were obtained for models with additional scalings,[3,4] such as letting the mass of the R.p. grow with time, so that the effect of possible recollisions (which carry a long-time memory) becomes negligible. In absence of additional scalings complete results could be obtained only for the equal mass one-dimensional case[5,6] and for a particular model for which the "R.p." (in this case actually a rod), tied to a straight line, moves under the action of collisions with a gas in the plane $\mathbb{R}^2$.[7,8] Some significant progress was however made for the one-dimensional gas with the mass M of the R.p. different from the common mass m of the other particles,[1] but the difficulty of estimating the contribution of the tail recollisions did not allow a complete proof of the Brownian limit.

In order to shed more light on the behavior of such systems some authors resorted to computer experiments,[9–11] and a first hint that the behavior for $M \neq m$ was not diffusive (Gaussian)[9] was contradicted by more accurate simulations,[11] so that by now the displacement of the R.p. can be assumed to be diffusive for all mass ratios. Computer simulations also showed that the dispersion changes in a peculiar way as the mass ratio $\frac{M}{m}$ varies, reaching a global maximum for $M = m$, which, as we have rigorous proofs for the equal mass case, is explicitely known ($D^* = \sqrt{\frac{2}{\pi}}$). In ref. 2 one can find a proof that this is an upper bound for all mass ratios, the lower bound being $D_* = \sqrt{\frac{\pi}{8}}$. The computer data show that, as the ratio $\frac{M}{m}$ moves away from 1, there is a clear fall-off of the dispersion on both sides, which for large ratios may go all the way to the lower bound D_* as $\frac{M}{m} \to \infty$. In the region $0 < \frac{M}{m} < 1$ the results of the first simulations[9] seemed to show that the dispersion, starting from values near D^* for $\frac{M}{m} = 1$, falls off, as $\frac{M}{m}$ decreases, to a local minimum, to go up again as $\frac{M}{m} \to 0$. It was natural to assume that the limiting value of the dispersion at $\frac{M}{m} = 0$ is D^*, so that one would have continuity of the dispersion at $M = 0$, as the system with $M = 0$ clearly behaves in the same way as for equal masses $M = m$.

The error bars in ref. 9 were however too large to allow definite conclusions on the behavior at low values of $\frac{M}{m}$. The corresponding picture in ref. 11, which has a better statistics, does not seem to be very much in agreement with the continuity hypothesis, but here again the data in the low-mass region are not enough to allow reliable conclusions. We are not aware of further results on this problem.

The aim of the present paper is to report some new computer simulations with more data in the region of low mass ratios and much larger

statistical samples than in ref. 11. The results presented here clearly indicate that there is no increase of the dispersion as $\frac{M}{m} \to 0$, and indeed the dispersion seems to decrease all the way as $\frac{M}{m} \to 0$. Hence there is no continuity of the dispersion at $\frac{M}{m} = 0$. We also report for comparison the corresponding results for the two-dimensional model considered in refs. 7 and 8, which is made of an infinitely thin rod, of mass M and length ℓ, which moves with its center on the x axis keeping an orthogonal position with respect to it, and interacts by elastic collisions with a free gas of particles of common mass m. The model is essentially one-dimensional, as the y-components of velocities are preserved. The additional dimension plays however an important role in the proofs, providing a rapid fall off of the memory, as the free gas particles move out of the interaction region in a finite time.

Our results show that for this model the dispersion as a function of the mass ratio behaves near the origin in the same way, i.e., it has a local minimum.

One can maybe argue that long memory effects, which are absent in the second model, do not affect the behavior of the dispersion in the neighborhood of $\frac{M}{m} = 0$.

2. DESCRIPTION OF THE MODELS AND OF THE COMPUTER SIMULATION

The main model that we consider is a one-dimensional particle system made of a particle of mass M ("Rayleigh particle," or "R.p.") and infinitely many particles of common mass m. Particles move freely except at the moments of collision, when they change velocity according to the laws of elastic collision. Namely the particles of equal mass m simply exchange velocities, whereas when the R.p., with velocity V, and a particle of mass m, with velocity v, collide they take, respectively, the outgoing velocities

$$\begin{cases} V' = \alpha V + (1-\alpha)\, v \\ v' = (1+\alpha)\, V - \alpha v \end{cases} \tag{1}$$

where $\alpha = \frac{m-M}{m+M}$.

Let Ω be the phase space of the system as seen from the R.p., with points $\omega = (V, Y)$ where V is the velocity of the R.p. and Y is a discrete subset of $\mathbb{R}^2$, giving positions and velocities of the other particles. Y has the property of being "locally finite," i.e., for any bounded measurable $\Lambda \subset \mathbb{R}^1$ the set $Y \cap (\Lambda \times \mathbb{R}^1)$ is finite. The time dynamics described above induces an evolution T^t on some regular subset $\Omega' \subset \Omega$.

For any inverse temperature β there is a unique Gibbs equilibrium state for the "system as seen from the R.p.," which, if $\rho > 0$ is the particle density, is a measure on Ω written as

$$\mu(d\omega) = \sqrt{\frac{M\beta}{2\pi}}\, e^{-\beta \frac{MV^2}{2}}\, dV\, \mathscr{P}_{\rho,\beta}(dY) \tag{2}$$

where $\mathscr{P}_{\rho,\beta}$ is the Poisson measure on $\mathbb{R}^2$ with intensity

$$\rho dq \sqrt{\frac{m\beta}{2\pi}}\, e^{-\beta \frac{mv^2}{2}}\, dv \tag{3}$$

As $\mu(\Omega') = 1$ for all choices of β, ρ (see ref. 1) there is no problem with the dynamics. The position of the particle at time t, assuming that it is located at the origin at the initial time $t = 0$, is given in terms of the dynamics on Ω by the explicit formula

$$Q(t;\omega) = \int_0^t V(T^\tau \omega)\, d\tau \tag{4}$$

In computer simulations we take the values $\rho = 1$, $\beta = 1$ and $m = 1$, as no significant dependence on such parameters is expected. As discussed in ref. 11, the simulation of the system requires the generation of Gaussian random variables (for the velocities) and of exponential random variables for the interparticle distances.

In carrying out the computation one has to follow a trajectory for long times, since by stopping the procedure and starting again one would introduce additional external randomness. The difficulty is of course that of keeping track of an increasing number of particles and of possible fast particles that come from far away. As in ref. 11 we introduce a "barrier," located at $\pm L$ where $L > 0$ is chosen in dependence of the maximal planned time of each run T, and is so large that the probability that for one of the runs in the sample the R.p. will ever get across the barrier by time T is negligible. At the barrier particles that are going to enter the interval $(-L, L)$ are "piled up," each of them labeled by its velocity v and entry time τ. The first particle that collides is determined by taking the minimum of the collision times of the R.p. with all particles in $(-L, L)$ and with the particles of the barrier. Let τ_* be such minimum. One should of course be sure that there is no fast particle that can enter the barrier and collide with the R.p. before time τ_*. This is ensured by checking that there are, at the barrier, particles with entry time larger that τ_*. If this is not the case we "fill up" the barrier with new particles. Clearly only particles with positive velocity are considered at $-L$, and particles with negative velocity at $+L$.

The joint distribution of the entry times and the absolute value of the velocities of the particles at the two points of the barrier is the same and, since we are dealing with "fresh particles" which have not yet collided, is independent of the situation at the initial time $t = 0$ in the interval $(-L, L)$ and is generated by the Poisson distribution $\mathscr{P}_{\rho,\beta}$. Simple computations show that the joint distribution of the entry time τ_1 and the absolute value of the velocity $u_1 = |v_1|$ of the first particle that enters at one of the points of the barrier has density

$$f(\tau_1, u_1) = \frac{1}{\sqrt{2\pi}} e^{-\frac{u_1^2}{2}} u_1 \, du_1 \, e^{-\frac{\tau_1}{\sqrt{2\pi}}} d\tau_1 \tag{5}$$

(Note that the density is properly normalized: $\int_0^\infty d\tau_1 \int_0^\infty du_1 \, f(\tau_1, u_1) = \int_0^\infty \frac{d\tau_1}{\sqrt{2\pi}} e^{-\frac{\tau_1}{\sqrt{2\pi}}} \int_0^\infty e^{-\frac{u_1^2}{2}} u_1 \, du_1 = 1$.)

By the properties of the Poisson distribution, the time differences with the particles that follow, $\tau_j - \tau_{j-1}$, $j = 0, 1, \ldots$, $\tau_0 = 0$ and the velocities $u_j = |v_j|$ of those particles are i.i.d. with the same distribution as τ_1, u_1.

The procedure for each run is the following. We first generate the number N_L of particles in $(-L, L)$ as an independent realization of a Poisson random variable with parameter $2L$. The particle positions are then determined as independent realizations of the uniform random variable in $(-L, L)$, and the particle velocities as independent realizations of the appropriate Gaussian variable. Particles on the barrier are assigned by a similar procedure. In computing the dispersion the time of each run is $T = 10{,}0000$ units, the position of the barriers is fixed with $L = 400$ and the sample N varies between 1,500 and 3,000.

The second model consists, as we said, of a rod of length ℓ and total mass M, moving in a plane in such a way that its central point moves on the x-axis, and its direction is always perpendicular to it. The rod moves under the action of elastic collisions with a gas of free particles with common mass m. At collision the y-component of the particle velocity is preserved, and the x-component changes according to the laws (1) where V, V' are the velocities of the rod (which are parallel to the x-axis, or "horizontal") before and after collision, and v, v' are the corresponding horizontal velocities of the gas particle. If V is the velocity of the rod, (q_1, q_2) the space coordinates and (v_1, v_2) the horizontal and vertical velocities, respectively, and Ω the phase space of the gas as seen from the rod, the Gibbs equilibrium measure is a measure on Ω written as

$$\mu(d\omega) = \sqrt{\frac{M\beta}{2\pi}} e^{-\beta \frac{MV^2}{2}} dV \, \mathscr{P}_{\rho,\beta}(dY) \tag{6}$$

where $\mathscr{P}_{\rho,\beta}$ is the Poisson measure on $\mathbb{R}^4$ with intensity

$$\rho\, dq_1\, dq_2 \sqrt{\frac{m\beta}{2\pi}}\, e^{-\beta \frac{mv_1^2}{2}}\, dv_1\, h(dv_2) \tag{7}$$

Here $h(dv_2)$ is the vertical velocity distribution, which is arbitrary, as the vertical velocity is preserved at collision. We take a discrete distribution for which the vertical velocity takes the four values $\pm\frac{1}{10}$ and $\pm\frac{1}{5}$ with equal probabilities. We set again $\rho = 1$, $m = 1$, and take $\ell = 10$.

This model needs of course a two-dimensional barrier, which is the boundary of the box $-\frac{\ell}{2} \leqslant q_2 \leqslant \frac{\ell}{2}$, $-L \leqslant q_1 \leqslant L$. The time of each run is $T = 1{,}000$, the position of the barrier varies between $L = 200$ and $L = 300$, and the sample N between 500 and 1,000.

3. ANALYSIS OF THE RESULTS

In all plots that follow vertical bars correspond to one standard error over the sample.

3.1. Brownian Behavior for Model 1

We first made a new check of the Gaussian behavior of the particle position $Q(t)$ for large t. The easiest check is linearity of the sample dispersion $\langle Q_t^2 \rangle$ with time. (Here and in the following sample averages are denoted by angle brackets $\langle \cdot \rangle$.) Figure 1 shows typical numerical results.

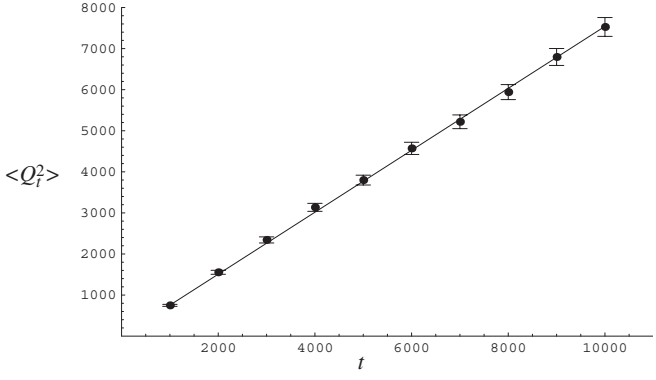

Fig. 1. Model 1. Plot of averages of Q_t^2, for $M = 2$, $N = 2,000$. The line is the linear best fit.

Table I. Results for Both the χ^2 and the K-S Test, Where M Is the Particel Mass, L the Exit Lenght, N the Sample Size, and k the Degrees of Freedom

M	L	N	χ^2	$\chi^2_{0.95,k}$	k	K-S test	$D_{N,0.05}$
0.02	40	10,000	41.83	42.6	29	0.0081	0.0136
0.5	40	5,000	90.03	100.85	79	0.0086	0.0192
0.5	70	5,000	92.34	102	80	0.0132	0.0192
0.5	100	10,000	72.93	88.2	68	0.0072	0.0136
1	40	5,000	100.84	124	100	0.0144	0.0192
1	70	5,000	68.44	99.7	78	0.0082	0.0192
1	100	5,000	97.73	100.85	79	0.0132	0.0192
2	40	5,000	84.32	99.7	78	0.0165	0.0192
2	70	5,000	55.15	88.22	68	0.0097	0.0192
2	100	5,000	57.68	88.22	68	0.004	0.0192

Following ref. 9 one can argue that a more significant check is perhaps that of the exit time distribution. For the standard Brownian motion the distribution of the exit time from the interval $[-1, 1]$ is given, following ref. 12, by the series

$$F(t) = 1 - \frac{4}{\pi} \sum_{j=0}^{\infty} \frac{(-1)^j}{2j+1} e^{-\frac{\pi^2}{8}(2j+1)^2 t}$$

We take different values of the length $2L$ of the interval, with center at the origin, for which we compute the exit time. The variable is rescaled by a factor $\frac{\sigma^2 t}{L^2}$. The results for both the χ^2 and the Kolmogorov–Smirnov test are reported in Table I. All results are compatible with the Brownian hypothesis.

3.2. Behavior of Dispersion with the Mass for Model 1

For a better description we report separately the results for different ranges of the mass ratio. They are given in Figs. 2a–c. The size of the sample can actually be considered to be $10N$, as we consider for each one of the N runs the increments of the displacement of the particle over time intervals of 1,000 units. (As a consequence of the Brownian limit such increments are approximately independent).

Figure 2a shows the behavior around the global maximum at $\frac{M}{m} = 1$. As in refs. 9 and 11, we have a neat peak at $\frac{M}{m} = 1$.

Figure 2b shows the behavior in the critical region near $\frac{M}{m} = 0$. It clearly indicates that the dispersion tends to a limiting value as $\frac{M}{m} \to 0$, which is around 0.73. The statistics is over a sample of 3,000 runs, except

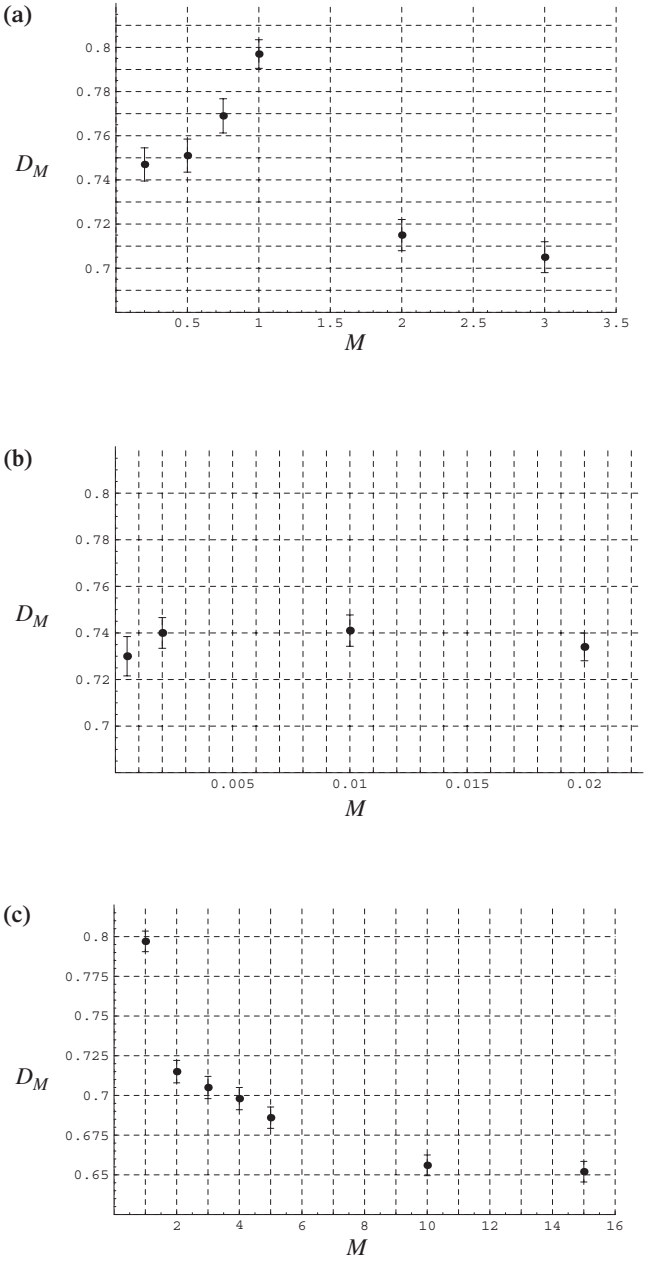

Fig. 2. (a) Model 1. Plot of D_M vs. M around the global maximum at $M = 1$. (b) Model 1. Plot of D_M vs. M in the critical region near $M = 0$. (c) Model 1. Plot of D_M vs. M for $M \geqslant 1$.

for the lowest value $M = 5 \cdot 10^{-4}$ for which the number of collisions is very large (and so are computing times) and the sample has been reduced to 1,500 runs. Figure 2c shows the behavior for large mass ratios.

3.3. Behavior of the Dispersion with the Mass for Model 2

For this model there is no reason to expect that as $\frac{M}{m} \to 0$ the value of the dispersion should tend to that for equal masses. The Brownian limit for this model was proved rigorously in ref. 7. As for the other model, we report separately the low mass behavior and that on the rest of the range.

Figure 3a gives the behavior over the whole range, which, in spite of the fact that error bars are larger, is clearly very similar to that of the previous model. And the same applies to the small mass behavior, on which we are mostly interested, as it is shown in Fig. 3b.

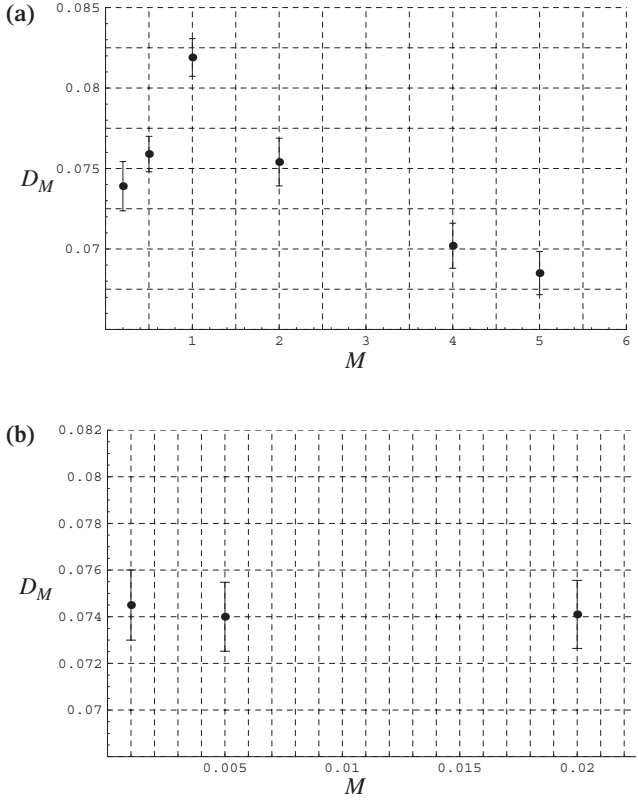

Fig. 3. (a) Model 2. Plot of D_M vs. M around the global maximum at $M = 1$. (b) Model 2. Plot of D_M vs. M for small mass.

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