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Numerical Evidence for Mass Dependence in the Diffusive Behavior of the "Heavy Particle" on the Line

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A numerical simulation shows that the diffusion constant of a test particle in a one-dimensional system of hard points depends on the mass of the test particle.

KEY WORDS: Diffusion constant; numerical simulation.

We consider the following dynamical system[1]: at time zero infinitely many point particles, all of mass $m=1$ (i.e., the bath), are distributed on $\mathbb{R}$ according to a Poisson distribution of density ρ, and a test particle of mass $m=M$ is posed at the origin. The velocities are distributed according to the Maxwell distribution for free particles, i.e.,

$$dP(v) = (\beta/2\pi)^{1/2} \exp(-\beta v^2/2)\, dv \tag{1}$$

for the bath particles, and

$$dP(V) = (\beta M/2\pi)^{1/2} \exp(-\beta M V^2/2)\, dV \tag{2}$$

for the test particle. The dynamics of the system is determined by Newton's law for elastic collisions among the particles.

Let $X(t)$, $V(t)$ be the position and the velocity of the test particle at time t; we are interested in computing the diffusion coefficient:

$$D = \lim_{t \to \infty} \langle X^2(t) \rangle / t = 2 \int_0^\infty \langle V(0)\, V(t) \rangle\, dt \tag{3}$$

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as a function of the mass M [averages in (3) are over the initial Gibbs distribution]. In the case $M=m=1$ (the "equal mass" case) a classical result gives $D=\langle|v|\rangle/\rho$.[1]. A corresponding explicit result for the unequal mass case is not known. However, some bounds are available. In fact in Ref. 2 it has been proved that

$$\frac{\langle v^2\rangle^2}{\langle|v|^3\rangle\rho}\leqslant D\leqslant\frac{\langle|v|\rangle}{\rho} \tag{4}$$

and one might conjecture that $D=\langle|v|\rangle/\rho$, i.e., that D is independent of M [this in fact appeared in a discussion between J. Lebowitz, S. Goldstein, and one of the authors (D.D.)].

In fact such is the case for the diffusion constant of a test particle moving in an infinite nearest-neighbor harmonic chain (for a recent treatment see Ref. 3). This leads then quite naturally to the conjecture that test particle diffusion in systems with pair potentials, allowing for harmonic approximation, is independent of the mass of the test particle.

Note that the diffusion in such one-dimensional system, where particles cannot separate over very large distances, arise only through the diffusive motion of the system as a whole: in particular, every particle of the system diffuses in the same way.

The dynamics of the one-dimensional hard point system is from a computational point of view very simple, and hence it is natural to test the first conjecture of mass independence of test particle diffusion by numerical simulation (simulation for the second conjecture is in preparation). We report here the result of a such a computer simulation which shows that the diffusion constant does in fact depend on the mass. In particular the diffusion constant of the test particle seems to have a maximum when its mass is equal to the mass of the bath particles. We expect this to be a special phenomenon occurring only due to the nonsmoothness of the hard point interaction.

Our computer simulations also suggest that the lower bound in (4) is achieved for very large M. This in fact leads to an explanation from which we also obtain a theoretical value for the large mass diffusion constant.

From (3), by change of variables, we obtain

$$D=2\int_0^\infty\langle\sqrt{M}\,V(0)\sqrt{M}\,V(Mt)\rangle\,dt \tag{5}$$

From Refs. 4 and 5 we know that essentially

$$\lim_{M\to\infty}\langle\sqrt{M}\,V(Mt)\sqrt{M}\,V(0)\rangle=\frac{1}{\beta}e^{-t\gamma}$$

with $1/\gamma\beta = \langle v^2\rangle^2/\langle |v|^3\rangle\, \rho \equiv D_\infty$, the lower bound in (4). Our simulation therefore suggests that the $\lim_{M\to\infty}$ may be exchanged with the time integral in (5).

From Ref. 4 we also know that the mechanical process $V(t)$ is for large M well approximated by a Markovian process $V^*(t)$ (on compact time intervals). Assuming this is true for all t, we are led to compute the diffusion constant D^* for the Markovian approximation $V^*(t)$. Now its generator is[4]

$$Ah(V) = \rho \int f(v)|v - V|\, h\left(V + \frac{2m}{M+m}(v - V)\right) dv - \lambda(V)\, h(V)$$

with $\lambda(V) = \rho \int f(v)|V - v|\, dv$. Thus

$$D^* = 2\int_0^\infty \langle V, e^{-tA} V\rangle\, dt = 2\left\langle V, \frac{1}{A} V\right\rangle,$$

and hence we look for a function $g(V)$ with $Ag(V) \cong V$, where $\cong$ means up to the order $O(1/M^2)$, considering $V = O(1/\sqrt{M})$. This is straightforward and yields

$$D^* \cong \frac{M+m}{2\rho m\langle |v|\rangle \beta M}\left(1 - \frac{3\sqrt{m}}{4M\langle |v|\rangle \sqrt{(2\pi\beta)}}\right) \tag{6}$$

and we observe that (for f Maxwellian)

$$\lim_{M\to\infty} = \frac{M+m}{2\rho m\langle |v|\rangle \beta M} = \frac{1}{2\rho m\langle |v|\rangle \beta} \equiv D_\infty$$

Furthermore, with our choice of m, β, and ρ (see following), Eq. (6) reads

$$D^* = \pi(1 - 3/(8M))\frac{M+m}{4Mm\rho} \tag{7}$$

See Table I for comparison with the computer results.

Table I. Values of the Diffusion Constant D at Different Masses M[a]

M	0.1	0.5	1.0	2.0	5.0	10.0	20.0
T	15.0	10.0	5.0	5.0	10.0	25.0	50.0
D	0.91 ± 0.03	0.98 ± 0.02	1.0 ± 0.02	0.96 ± 0.02	0.84 ± 0.02	0.81 ± 0.02	0.79 ± 0.02
D^*				0.957	0.872	0.831	0.809

[a] T is the time (in units of the mean collision time) used for the computation; D^* is the result obtained from the Markovian approximation (6).

Our numerical simulation in order to compute D is straightforward. A number n of bath particles are distributed on the interval $[-L, L]$ according to a uniform distribution with density $\rho = 1$, and the initial velocities are given by (1). We fix the temperature $1/\beta = \pi/2$ (then we have $\langle |v| \rangle = 1$, $\langle v^2 \rangle = \pi/2$, $\langle |v|^3 \rangle = \pi$). The test particle is placed at the origin and its velocity is extracted from (2). Then we compute the motion of the test particle up to a large enough time T (see the following) directly using the law of collisions. No integration error occurs in the construction of the trajectories, because the dynamics is exactly solvable. The process is iterated for a large sample of independent initial configurations. For each trajectory of the sample we evaluate $X(t)$ and the corresponding velocity $V(t)$ on the time interval $[0, T]$. The averages in (3) are then performed over the collected data. In all our runs we use 100,000 independent trajectories (so that the statistical error is less than 1%). We note that the algorithm to evaluate the averages is not the one usually employed in molecular dynamics (MD) calculations, where a single long time-mechanical trajectory is used to average over many time-origins. In fact for this simple system it is possible to exact independent initial configurations directly from the exact Gibbs distribution: unlike usual MD calculations there is therefore no persistence of correlation between subsequent initial configurations.[6] Another advantage of taking ensemble averages instead of time averages is that is is sufficient to follow the trajectory only for the time T which is necessary to observe the linear behavior of $\langle X^2(t) \rangle$ and to correctly integrate $\langle V(0)\, V(t) \rangle$ (T obviously depends on M). This time is (of course) much shorter than the time used in MD for statistical reasons.

We found that for such time T it is possible to use a large enough system to make the test-particle motion insensible to the boundary conditions. We used a free system, i.e., neither walls nor periodic boundary conditions were imposed. To make sure that the size of the system was suitable, we monitored the rate of the average number $\langle c(t) \rangle$ of test-particle collisions at time t: for systems with $350 \leqslant n \leqslant 700$, $d\langle c \rangle/dt$ starts decreasing at times which are always greater than T. This behavior is shown in Fig. 1 for the case $M = 10$. We also verified that up to time T the trajectory of the test particle computed using periodic boundary conditions is the same as that computed in the free system.

The diffusion coefficient has been computed both by means of the integral of the autocorrelation function of the velocity and by measuring the slope of the linear region of the mean square displacement. Figure 2 shows $\langle X^2(t) \rangle$ in the case $M = 10$: as can be seen, the noise is negligible. The values of the diffusion coefficient for different test-particle masses are listed in Table I. The values of D obtained by $\langle X^2(t) \rangle$ and $\langle V(0)\, V(t) \rangle$ agree within the error reported in the table. The numerical value for $M = 1$

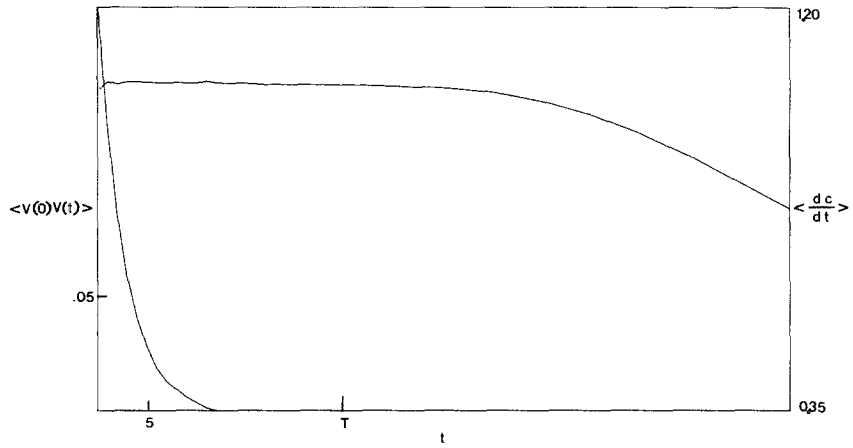

Fig. 1. Average rate of test-particle collisions $d\langle c\rangle/dt$ as function of time in the case $M=10$ and $n=350$ (t is in units of the mean collision time). T is the time used to compute D. The decay of the velocity autocorrelation function is also plotted for comparison.

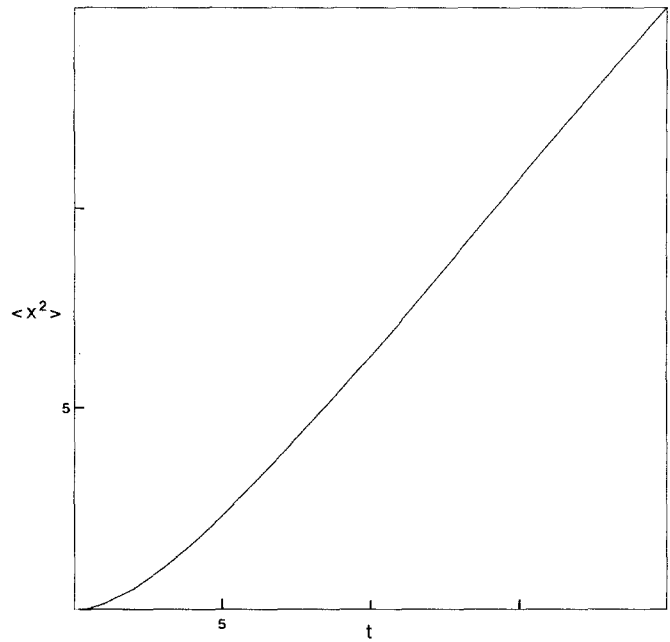

Fig. 2. Mean-square displacement vs. time in the case $M=10$ and $n=350$ (t is in units of the mean collision time).

coincides with the theoretical result $D = 1$. For $M \neq 1$ all the values of D are within the bounds (4) (with our choice of β and ρ the bounds are $\pi/4 \leqslant D \leqslant 1$); however, they are different from 1. We also note that the value found in the case $M = 20$ is very near to the theoretical lower bound $D = \pi/4 = 0.7854$.

Figure 3 illustrates, in the "heavy mass" case, the behavior of the autocorrelation function. It appears that in this case the autocorrelation functions decays without oscillation from positive values to zero. The decay shows a twofold behavior: at the beginning it is clearly exponential, and then it seems to follow a powerlaw. This is visible in the figure, where lines corresponding to the decay t^{-3} are plotted for comparison (t^{-3} is the decay to zero from negative values in the equal mass case[1]). The power-

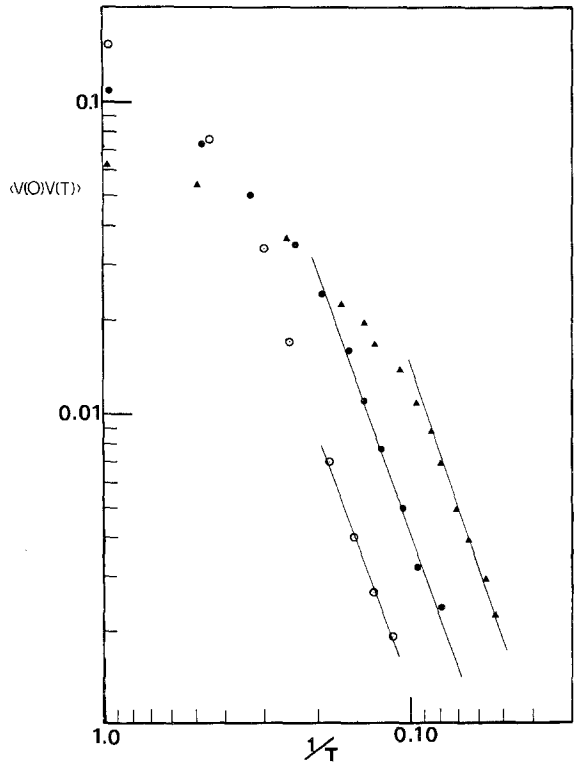

Fig. 3. The decay of the velocity autocorrelation as a function of time (in units of the mean collision time) for three values of the mass M of the test particle on a log-log plot. The open circle, closed circle, and triangle refer to $M = 5$, $M = 10$, and $M = 20$, respectively. The straight lines are drawn with a slope corresponding to t^{-3}. The system has 700 bath particles and the averages are performed over 100,000 initial configurations.

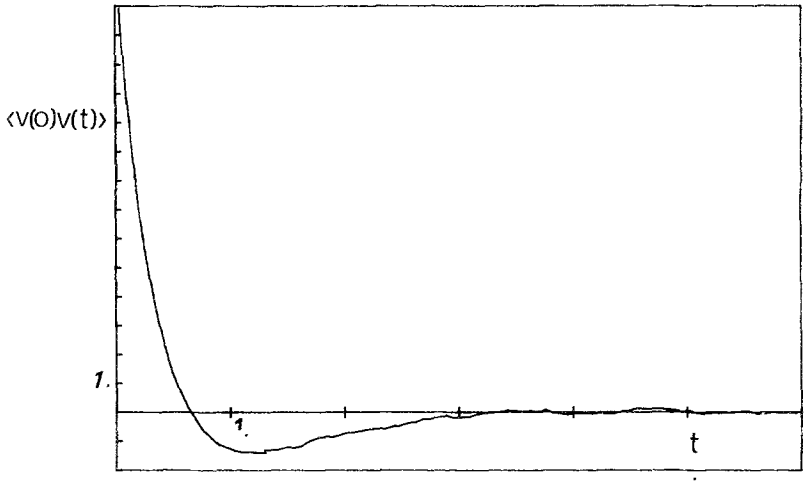

Fig. 4. Deay of $\langle V(0)\, V(t)\rangle$ for $M = 0.1$.

law decay starts at times which are large enough to give only a negligible contribution to the value of D.

Figure 4 shows the behavior of $\langle V(0)\, V(T)\rangle$ in a "light mass" case. For $M \leqslant 1$ the autocorrelation function has a negative minimum and seems to present damped oscillations about zero: the noise, though, is in this case higher so that a more accurate analysis is numerically difficult.

The computations were performed on the CRAY X-MP 12 at CINECA (Casalecchio-Bologna).

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