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Diffusion and Einstein Relation for a Massive Particle in a One-Dimensional Free Fas: Numerical Evidence

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A computer simulation is used to investigate the motion of a marked particle of mass M in a free gas of particles with mass $m = 1$, for large times. Previous results seem to indicate a non-Wiener behavior for the rescaled trajectory when $M \neq m$. The results reported here, with better statistics, are compatible with the Wiener hypothesis. The Einstein relation between mobility and diffusion coefficient is also investigated. The results indicate that it holds both for $M = m$ and for $M \neq m$.

KEY WORDS: Brownian limit; Einstein relation; computer simulation; tagged particle in free gas.

1. INTRODUCTION

In recent years increasing attention has been devoted to the study of mechanical models of Brownian motion. It is now well understood that Brownian motion can be obtained just by space-time rescaling, without changes in the dynamics. A simple model for which the derivation can be carried out in a mathematically rigorous way was introduced by Harris[1] and studied by Harris and Spitzer.[2] It is the motion of a marked particle in a one-dimensional gas of identical ideal particles undergoing only elastic collisions. From the point of view of mechanics it is a very special model, since all velocities are preserved. This is actually the reason why the model is tractable, and one can prove that the normalized displacement of the marked particle is asymptotically Wiener if the system is in an equilibrium state. (For other initial states one can get a different results; see ref. 3.)

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The next obvious step is that of allowing the mass of the marked particle M to be different from the common mass m of the other particles. In this case velocities change when the marked particle collides, and the mathematical investigation of the model is much harder. Nevertheless, some rigorous results have been recently obtained by Sinai and Soloveichik[4] and Szász and Tóth.[5] They considered a state for which the marked particle with mass M (hereafter called "massive test particle" or m.t.p.) is at the origin, with velocity V distributed according to a Maxwell distribution with inverse temperature β, and the distribution of the other particles (with mass m, hereafter called "light" particles, though they may be heavier) is independent of V and is a free gas distribution with the same temperature. The state constructed in this way is an equilibrium state with respect to the composition of the usual dynamics with the shift that brings back the m.t.p. at the origin (see refs. 4 and 5 for details). It was proved in refs. 4 and 5 that the normalized displacement $\xi_t \equiv q_0(t)/\sqrt{t}$ of the m.t.p. is asymptotically equal to the difference of two Gaussian variables, which, however, are in general dependent. Also, bounds for the limiting variance of ξ_t were obtained.

The question of whether ξ_t is asymptotically Wiener remains open, and computer investigations were made in order to get some insight. In a recent paper[6] it was claimed that the process ξ_t is not asymptotically Gaussian for $M \neq m$. Other numerical evidence[7] apparently supports the opposite conclusion, though the method used here in computing the distribution of ξ_t is doubtful, since, in contrast to the method used in ref. 6, only short runs were allowed. This can hide the effects of long-time tails, which could be responsible for the possible non-Wiener character of the process.

In order to get a definite answer, we performed a numerical simulation, which is similar in method to that of ref. 6, but was carried out for longer times and with better statistics. In addition to studying the distribution for fixed times, we also compared the exit time distribution with the Wiener one. It is reasonable to expect that the exit time distribution is a more reliable test, since it depends on the global behavior of the trajectory.

We also tested the validity of the Einstein relation between mobility and dispersion, when the m.t.p. is subject to a small constant force. Validity of the Einstein relation may be considered as additional evidence of the diffusive character of the motion.

We set the inverse temperature β equal to 1, the light particle density equal to 1, and $m = 1$. We considered several values of the mass M, both larger and smaller than 1. Our results can be summarized as follows.

The dispersion of the normalized displacement ξ_t depends on the mass M in a way that is in accordance with the results of ref. 6, except for small values of M (Section 3). The hypothesis of a Gaussian asymptotic distribution for ξ_t cannot be rejected for all values of the mass M that were considered (Section 3). Moreover, the exit time distribution is in accordance with the Wiener exit time distribution.

The Einstein relation has been tested for $M = 0.5$, 2, and 4, and for $M = m = 1$, for comparison. The computer data show that it holds in all cases within the presumable statistical errors (Section 4). As additional evidence, one might consider the Gaussian-like decay of the tail of the distribution of the ξ_t found in ref. 3.

In conclusion, we may say that our results support the hypothesis that the process $\xi_T(t) \equiv \sqrt{t}\, \xi(tT) = q_0(tT)/\sqrt{T}$ is, for large T, asymptotically Wiener for $M \neq m$.

2. NUMERICAL METHOD

The initial configuration was obtained in the following way. We set the m.t.p. at 0 with a velocity chosen at random, according to the appropriate distribution (with density $[\exp(-v^2/2M)]/(2\pi M)^{1/2}$), and generated the random positions of the light particles in a fixed interval $I_L = (-L, L)$ by simulating a Poisson point process with intensity $\rho = 1$ (i.e., distances between neighboring particles were chosen independently according to the exponential distribution with parameter $\rho = 1$). Finally, the light particles were given standard Gaussian independent velocities.

To observe long runs, one has to find a way of taking into account the random flux of the particles that enter the interval I_L from the outside. If this is done, the evolution can go on until the m.t.p. reaches $\pm L$, that is, assuming diffusive behavior, for a time of $O(L^2)$. Our choice of L is fixed and is $L = 400$.

Since for our equilibrium state the distribution of the light particles is a free gas equilibrium state, we know the distribution of the positive (negative) velocity particles that enter at $+L$ $(-L)$. In the variables u, τ, where u is the absolute value of the velocity and τ the entrance time, the distribution has density

$$f(u, \tau) = (1/\pi) \exp(-u^2/2) \exp[-\tau/(2\pi)^{1/2}]$$

For each boundary point $\pm L$ we generated a finite sequence of random entrance times and velocities, which were kept in a "waiting list": a particle with entrance time τ is taken into account only for times $t \geq \tau$.

To spare computer time, we reduced the number of particles that the computer takes into account to determine collisions by the following device. We take an inner interval I_l with center at 0 and semilength $l < L$

("barrier") around the position of the heavy particle, i.e., an inner interval of length $l<L$. The particles in $(-L, L)$ and in the waiting list are classified as "in particles" (those that are inside the barrier or are going to be inside within some fixed time $\bar{t}$, and "out particles" (the other ones). At time $\bar{t}$, or at the first time the m.t.p. reaches the barrier, the evolution is stopped and the barrier is updated as follows. We take a new interval I' with center at the new position of the m.t.p., and take as "in particles" those that are inside I' or are going to be within time $\bar{t}$. The semilength l' of I' is the minimum between l and the distance of the position of the m.t.p. from the border $\pm L$. Of course, the waiting list is always kept long enough so that the last particle will enter $(-L, L)$ at a time larger than $\bar{t}$. The barrier is just a way of keeping track of the evolution and adds no new stochasticity. For our choice of L, which was fixed at $L=400$, we could always follow the initial configuration up to times of the order of 10,000, i.e., the m.t.p. never reached the border $\pm L$ before this time.

Computations were made on a Microvax II. The influence of the random number generator is briefly discussed in the concluding remarks.

3. DEPENDENCE OF THE DIFFUSION COEFFICIENT ON THE MASS AND TEST OF THE WIENER CHARACTER OF THE PROCESS

3.1. Diffusion Coefficient As a Function of the Mass

The asymptotic diffusion coefficient

$$D_M \equiv \lim_{t\to\infty} \mathbf{E}\,\frac{\xi_t^2}{t}$$

was computed in the following way. We took runs for a time 10^4 and recorded the values of ξ_t at the times $t_i=iT$, $T=10^3$. We then computed the sample averages of the quantities $(\xi_{t_i}-\xi_{t_{i-1}})^2/T$ and expressed D_M as the average of $D_M^{(i)} \equiv (\xi_{t_i}-\xi_{t_{i-1}})^2/T$, $i=1,\ldots, 10$ (ergodic average). The sample number N is in all cases larger than 10^3. Computer data show that the correlation coefficient between different increments $\xi_{t_i}-\xi_{t_{i-1}}$ is very small, of the order of 10^{-3}. Table I shows the computed values, with the standard deviation (the square root of the empirical variance of $D_M^{(i)}$) and the number of runs N. The behavior of the sample averages of $\xi_{t_i}^2$ as a function of t_i is linear with very good approximation, as shown by Fig. 1, corresponding to the case $M=2$, $N=1{,}000$.

The behavior of the diffusion coefficient D_M as a function of M is shown in Fig. 2. The theoretical lower and upper bounds for our choice of the parameters are $(\pi/8)^{1/2}$ and $(2/\pi)^{1/2}$. There is clear evidence that D_M

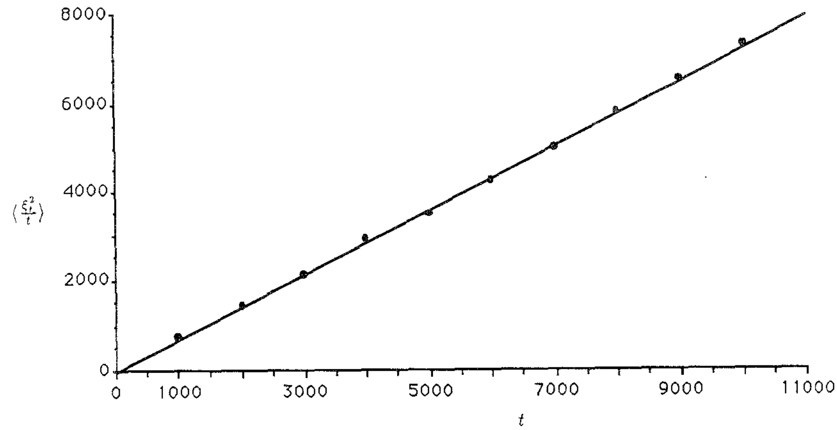

Fig. 1. (●) Plot of the averages over 10^3 runs of ξ_t^2/t, for $M=2$. The line is the linear fit.

depends on the mass and tends to the lower bound for large M. Our results differ from those of ref. 6 in that for small values of the mass we do not observe a tendency to the upper bound D_1. Instead, it appears that for $M=0.2$ and $M=0.02$, D_M is lower than for $M=0.5$, and it may be that for $M \to 0$, D_M does not tend to the value for $M=0$, which should be the same as for $M=1$. This would be hard to check, however, because with our computation method small values of M require, very long computer times.

3.2. Test of the Gaussian Character of $\xi(t)$

We have tested the Gaussian character of $\xi(t)$ for large times by making a χ^2 test. Table II reports the computed values of χ^2 for 48 degrees

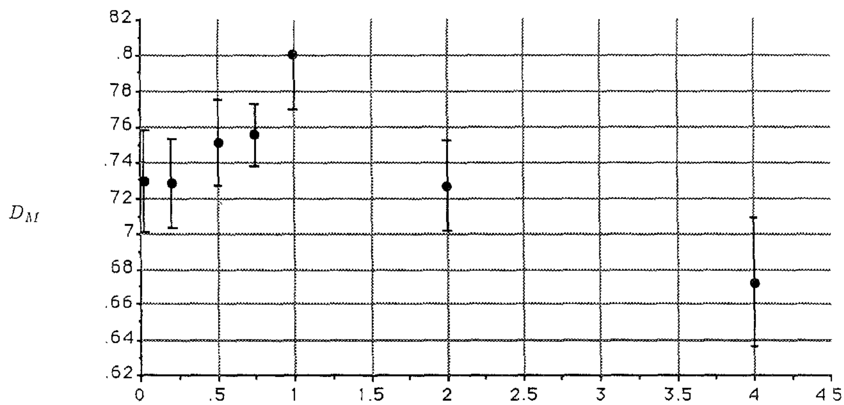

Fig. 2. Plot of D_M vs. M. Error bars correspond to one standard deviation.

Table I

M	0.02	0.2	0.5	0.75	1	2	4
D_M	0.729 ± 0.028	0.728 ± 0.025	0.751 ± 0.024	0.755 ± 0.018	0.8 ± 0.031	0.727 ± 0.025	0.673 ± 0.036
N	1200	2000	2000	2000	2000	1000	1000

Table II

		χ^2 for given value of t									
M	N	1000	2000	3000	4000	5000	6000	7000	8000	9000	10,000
0.5	2000	47.34	48.09	41.77	66.35	48.07	42.32	44.79	49.56	51.90	41.45
0.75	2000	58.02	55.12	36.16	39.86	48.14	49.10	43.22	48.93	46.84	55.78
1	2000	41.29	62.78	45.21	38.32	43.57	36.74	37.19	49.70	54.32	37.12
2	1000	48.73	33.76	45.88	48.82	50.67	55.40	41.03	31.29	47.17	42.07
4	1000	52.11	67.28	36.33	38.19	36.72	53.77	53.25	44.67	45.62	41.47

of freedom for different choices of the mass M and of the time t. The number N of runs varies, but $N/48$ is large enough in all cases. The dispersion of the reference Gaussian distribution is taken equal to the computed one, given by Table I.

To estimate the significance of the results, one should compare with the reference value χ^2_{1-p} (for 48 degrees of freedom), defined by the equality $P(\chi^2 > \chi^2_{1-p}) = p$, where P corresponds to the reference (Gaussian) distribution for $\xi(t)$. Here are some values: for $p = 0.05$, $\chi^2_{1-p} = 65.15$; for $p = 0.1$, $\chi^2_{1-p} = 60.9$; and for $p = 0.5$, $\chi^2_{1-p} = 47.33$.

3.3 Test of the Exit Time Distribution

For the one-dimensional Wiener process starting at 0 the distribution of the exit time from the interval $[-1, 1]$ is known[8] to have a distribution function

$$F(t) = 1 - \frac{4}{\pi} \sum_{j=0}^{\infty} \frac{(-1)^j}{2j+1} \exp\left[-\frac{\pi^2}{8}(2j+1)^2 t\right]$$

We have tested the hypothesis that $F(t)$ is the distribution of the exit time from the interval $[-50, 50]$, properly rescaled. The test is very sensitive to the value of the diffusion coefficient that is assumed for the reference Wiener process. For $M = 1$ we took the theoretical value of D_M. For $M = 0.5$, 2, 4 we looked for the value of D_M, around the computed value of Table I, which gave the best χ^2 value. It turns out that the value of D_M obtained in this way is always within one standard deviation from the value of Table I. In addition to the χ^2 test, we also made a Kolmogorov–Smirnov test for the same value of D_M.

In Table III we report on the left the results of the χ^2 test and the values of $\chi^2_{0.95}$ for k degrees of freedom, denoted by $\chi^2_{0.95,k}$. On the right we give the results of the Kolmogorov–Smirnov (KS) test and the critical values $D_{N,0.05}$, where N is the number of observations and 0.05 is the significance level. For $M = 0.5$, 2, 4 the test was made with a reference

Table III

M	D_M	N	χ^2	$\chi^2_{0.95,k}$	k	KS test	$D_{N,0.05}$
0.5	0.746	9941	68.47	100.76	79	0.007	0.014
1	0.798	3082	70.554	101.9	80	0.015	0.024
2	0.732	3121	62.11	100.76	79	0.02	0.024
4	0.657	3140	88.58	98.49	77	0.02	0.024

Gaussian distribution with the computed empirical dispersion given by Table I. It is clear that, with a level of significance of 5%, the Wiener hypothesis cannot be rejected.

4. CHECK OF THE EINSTEIN RELATION

The "Einstein relation" is a proportionality law discovered by Einstein between the mobility σ of the test particle for vanishing force and the diffusion coefficient D:

$$\sigma = \lim_{E \to 0} \frac{\mu(E)}{E} = \frac{\beta D}{2}$$

Here $\beta = 1/kT$ is the inverse temperature, $\mu(E) = \lim_{t \to \infty} [\mathbb{E}(q_0^E(t))/t]$ is the drift, with applied esternal field E, and $D = \lim_{t \to \infty} [\mathbb{E}(q_0(t))^2/t]$ is the diffusion coefficient computed for the equilibrium measure ($E = 0$).

The validity of the Einstein relation is believed to be connected to diffusive behavior for zero force, at least at the level of physical heuristics. The mathematical analysis was carried out only for some simple models, for which one can find a unique stationary nonequilibrium state for the environment.[9] If the stationary nonequilibrium state is not known or is not unique, it seems that there are problems with computer simulations, since the drift might depend on the choice of the initial distribution. The careful analysis carried out in ref. 9 shows, however, that the initial distribution should be the equilibrium state for zero field ($E = 0$). That is, the stationary nonequilibrium state that is relevant for the Einstein relation

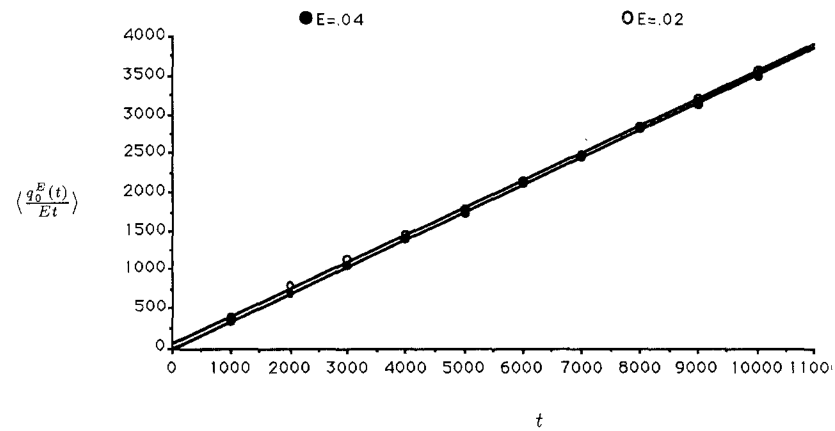

Fig. 3. The two lines are the best fit of the points that correspond to the sample average of $q_0^E(t)/Et$ for $E = 0.04$ and $E = 0.02$. The sample number is $N = 500$.

Table IV

M	$E/M=0.01$	$E/M=0.005$	$E/M=0.0025$
2	0.354	0.347	0.372
4	0.351	0.357	0.277

is the one obtained as the limit as $t \to \infty$ of the evolution of the equilibrium ($E=0$) state.

So for checking the Einstein relation the initial distribution was generated exactly as described in Section 2. The results show that the linear behavior for the displacement sets in fairly soon for the values of E that were considered. (One can in fact expect that relaxation to the unique stationary state does not depend significantly on E for small E.) Moreover, the average displacement divided by E, $\mathbb{E}(q_0^E(t))/E$, is linear in t, and independent of E for small E.

Figure 3 shows the plot of the average value (over the sample) $\langle q_0^E(t)/E \rangle$ for $M=4$ and $E=0.04$, 0.02. Table IV shows the results for the mobility, computed as the sample average $\langle \sum_i [q_0^E(t_i)/Et_i] \rangle$, for $M=2$, 4 and different values of E. The standard deviation corresponds to the empirical dispersion of $q_0^E(t)/t$, which for our values of E turns out to be equal to the dispersion D_M of Table I, i.e., for the equilibrium state with $E=0$, within the statistical errors.

5. CONCLUDING REMARKS: TEST OF THE RANDOM NUMBER GENERATOR

The reliability of computer simulations of random processes depends of course on how good the random number generator is. We used the random number generator of Microvax II, giving independent random numbers uniformly distributed between 0 and 1.

It is important for us that long sequences of outputs of the generator can be considered as independent. We tested the independence of sequences by a permutation test for groups of four variables.[10] For a sequence of 8×10^5 outputs, the result of a χ^2 test (with 23 degrees of freedom) gives a χ^2 value of 22.654, indicating that the generator is good enough for our purposes.

One can also expect that the distribution of the "random output" ξ given by the generator is not accurate near the boundary points 0 and 1. A way of testing the accuracy near the boundary points, as well as independence, is to check the arcsine distribution for the fraction of the integers k

for which the sum $\sum_{j=1}^{k} (\xi_j - 1/2)$, $k = 1,..., N$, is positive, for large N. The arcsine distribution gives a large weight to boundary points, and enhances possible anomalies in the distribution of long sequences af ξ_j close to the extreme points. A test made for $N = 1.5 \times 10^6$ showed that the weight of the region near the boundary points is what it should be. In particular, the distribution near the boundary points is symmetric with very good accuracy. A χ^2 test for 100 degrees of freedom gives 110.79 ($\chi^2_{0.95,100} = 124.3$).

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REFERENCES

1. T. E. Harris, Diffusion with "collisions" between particles, *J. Appl. Prob.* **2**:323 (1965).
2. F. Spitzer, *J. Math. Mech.* **18**:973 (1969).
3. P. Major and D. Szász, On the effect of collisions on the motion of an atom in $\mathbb{R}^1$, *Ann. Prob.* **8**:1068–1078 (1980).
4. Ya. G. Sinai and M. R. Soloveichick, One-dimensional classical massive particle in the ideal gas, *Commun. Math. Phys.* **104**:423–443 (1986).
5. D. Szász and B. Tóth, Bounds for the limiting variance of the "heavy particle" in $\mathbb{R}^1$, *Commun. Math. Phys.* **104**:445–455 (1986).
6. M. L. Khazin, Investigation of the diffusion of a massive particle in a one-dimensional ideal gas, *Teoret. Mat. Fiz.* **71**(2):299–303 (1987) [in Russian].
7. E. Omerti, M. Ronchetti, and D. Dürr, Numerical evidence for mass dependence in the diffusive behavior of the "heavy particle" on the line, *J. Stat. Phys.* **44**:339–346 (1986).
8. P. Erdős and M. Kac, *Bull. Am. Math. Soc.* **52**:292–302 (1946).
9. P. Ferrari, S. Goldstein, and J. L. Lebowitz, *Statistical Physics and Dynamical Systems: Rigorous Results* (Birkhauser, Boston, 1985).
10. D. E. Knuth, *The Art of Computer Programming*, Vol. 2, *Seminumerical Algorithms* (Addison-Wesley, Reading, Massachusetts, 1981), p. 64.