ON THE DYNAMICAL DISEQUILIBRIUM OF INDIVIDUAL PARTICLES

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In one of the most stimulating papers read at the Fourth Berkeley Symposium, S. Ulam [1] raised the question of how rapidly an assembly of colliding elastic particles would settle down into its equilibrium state. If initially the assembly consists of fast and slow particles, it is a familiar principle that the fast particles will tend to slow down and the slow particles to speed up until, viewed macroscopically, energy is shared uniformly among the assembly. Ulam reported on Monte Carlo studies with a high-speed computer, which tracked the histories of individual particles in such an assembly in regions of one or more dimensions. It was found that the energies of individual particles fluctuated very irregularly, though it might be hoped that, if the computation could have been carried on long enough, individual energies would eventually approach some neighborhood of their expected equilibrium values. The purpose of the present note is to handle theoretically one of the simpler one-dimensional cases, considered by Ulam, and to show that individual energies do *not* approach their equilibrium values: in short, the fluctuations observed on the computer will persist indefinitely, however long the computation. I cannot see any good reason why a similar failure to attain individual equilibrium should not also hold in a real system in three dimensions.

The following discussion also shows that the fluctuations of energy occurring in a fixed region of space are qualitatively different from the fluctuations occurring in a fixed set of particles. The former are less irregular than the latter, but even so do not settle down to equilibrium. The type of disequilibrium treated in the present paper is a persistent instability, to be contrasted with the transient instability discussed at length in the literature. Many papers in this literature assume that instability will be transient and proceed, *on this assumption*, to determine the relaxation times of this transience. For a review of the literature and a bibliography of 157 papers, see [2]; references [3] through [8] provide a selection of subsequent articles.

Ulam considered, among other matters in his talk, the following idealized one-dimensional situation. A weightless elastic particle is constrained to move on a straight line between a reflecting barrier and a heavy particle, which oscillates along the same straight line. Each time the weightless particle strikes the heavy one its speed, due to the elastic collision, is increased or diminished by twice the speed of the heavy particle according to whether the two particles were moving in opposite or the same directions immediately prior to impact. The motion of the heavy particle is unaffected by the collision. The problem is to determine how the motion of the weightless particle at various subsequent instants of time will depend upon its initial position and velocity. Heuristically one might suppose that the heavy particle will try to share its energy with the other particle, which being weightless will thereby be progressively accelerated to higher and higher speeds without limit. An alternative plausible argument notices that head-on collisions occur more frequently than overtaking ones, because of the higher relative velocity, and concludes that the weightless particle will, apart from minor relapses, exhibit a general tendency to gather speed indefinitely. As far as I could discover from subsequent conversations, all those in Dr. Ulam's audience, who had any feelings on this matter, were agreed that the particle would possess this general tendency to gather speed, though there was some divergence of opinion on the possible rate of gain of speed. A majority believed that the speed would increase linearly with time, while a minority (among whom I have to number myself) were inclined to a variety of slower increases, say logarithmically with time. It will appear from the following analysis that the majority were right, in that the expected speed does increase linearly with time: but there are also a number of amusing and at first sight paradoxical concomitant effects. For instance, the weightless particle returns to its initial speed infinitely often, and indeed spends a greater fraction of its time at any given small speed than at any given greater speed. If the process continues for a long duration T, the expected time spent in any prescribed speed zone is asymptotically proportional to $\log T$; and the constant of proportionality depends only upon the width of the zone and in no way on its mean value. These effects are less surprising when one knows that, although the expected speed of the weightless particle increases linearly with time, the variance of its speed increases quadratically with time. In short, the fluctuations in speed get wilder and wilder as time passes.

But it must here be stated that the conclusions quoted above apply to a slightly modified version of Ulam's problem. The primary purpose of the modifications is to simplify the analysis; but, by a very fortunate chance, these same modifications tend to make the formulation of the problem less idealized and much more like the real physical situation, although the restriction to motion in one dimension remains. For computational simplicity, Ulam supposed that the heavy particle oscillated with a saw-tooth wave form. This supposition is also convenient in the analytical treatment. However, for analytical convenience I shall suppose that, at successive collisions, the light particle strikes not a single heavy particle, as in Ulam's formulation, but a succession of different heavy particles, each performing the same saw-tooth oscillation, but with phases which are random and independent of each other. This modification removes the Diophantine difficulties which beset the original Ulam problem, and it also comes nearer to the physical situation in which each individual particle collides with a collection of more or less uncorrelated particles. The other modification, adopted for analytical simplicity, is to suppose that at any instant the weightless particle will collide with a heavy one according to a Poisson process whose parameter is linearly dependent upon the velocity of the weightless particle. Again, this simplification has the merit of reproducing the usual physical system with exponentially distributed free distances between particles.

With these simplifications we may now write down equations for the process. Suppose we choose units of distance such that the velocity of a heavy particle is always $\pm 1/2$. Thus if the period of oscillation is $2t_0$, the complete amplitude (crest to trough) of the saw-tooth wave will be $t_0/2$; see figure 1, in which posi-

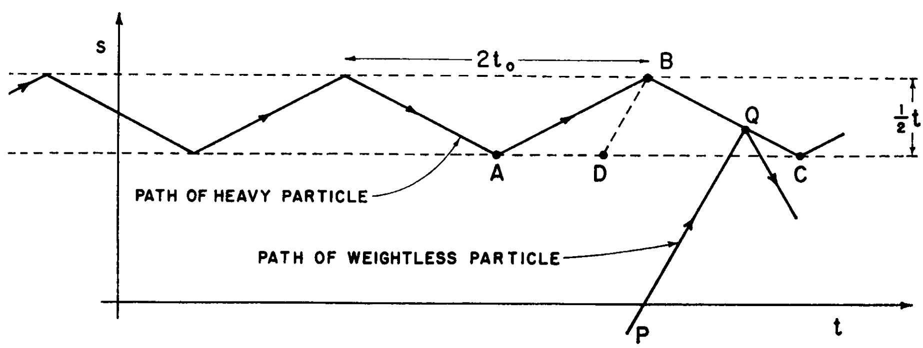

FIGURE 1
Position s plotted against time t.

tion s is plotted against time t. Suppose that before impact the velocity of the weightless particle is v, so that the slope of the line PQ in figure 1 is v. If the collision point Q occurs on a segment such as BC, where the velocity of the heavy particle is $-1/2$, the weightless particle will rebound with speed $v + 1$; whereas, if Q lies on AB, the weightless particle will rebound with speed $v - 1$. By drawing a line BD parallel to QP, and noting that the phase of the saw-tooth oscillation is uniformly random with respect to the path of the weightless particle, we see that the probabilities of v going to $v + 1$ and $v - 1$ respectively are in the ratio $DC{:}AD$. The geometry of figure 1 yields $AD = t_0(1 - 1/2v)$ and $DC = t_0(1 + 1/2v)$. Hence, given that a collision occurs, we have the conditional probabilities

$$(1)\qquad \begin{aligned} P\{v \to v + 1\} &= \frac{1}{2} + \frac{1}{4v} = \frac{2v + 1}{4v}, \\ P\{v \to v - 1\} &= \frac{1}{2} - \frac{1}{4v} = \frac{2v - 1}{4v}. \end{aligned}$$

The above working requires some minor modifications if $v < 1/2$; but, for simplicity, we shall presently adopt initial conditions which ensure that $v \geqq 1/2$ and accordingly we may regard equation (1) as valid.

Next we have to take account of the probability of a collision. We have postulated above that this shall be according to a Poisson process with parameter proportional to the velocity of the weightless particle; and, by a suitable choice of the units of time (or what comes to the same thing, by a suitable unit for the mean free path), we may take the constant of proportionality to be 2. Thus the probability that a collision will occur in an elementary interval of time dt is

$$2v\,dt. \tag{2}$$

By combining (1) and (2), we see that, if the weightless particle has present velocity v, the probabilities relating to an instant dt later are respectively

$$\begin{aligned} P\{v+1|v\} &= \frac{1}{2}(2v+1)\,dt, \\ P\{v|v\} &= 1-2v\,dt, \\ P\{v-1|v\} &= \frac{1}{2}(2v-1)\,dt. \end{aligned} \tag{3}$$

Thus (3) provides the infinitesimal transition probabilities of a Markov process.

For convenience we will suppose that the weightless particle starts initially with velocity $v = 1/2$. Its velocities at all subsequent instants then belong to the set $v = 1/2 + k$, where k runs through the states $k = 0, 1, 2, \cdots$. In terms of these states, the transition probabilities (3) become

$$\begin{aligned} P\{k+1|k\} &= (k+1)\,dt, \\ P\{k|k\} &= 1-(2k+1)\,dt, \\ P\{k-1|k\} &= k\,dt. \end{aligned} \tag{4}$$

Let $p_k(t)$ denote the probability that the weightless particle is in state k at time t, where $t = 0$ specifies the initial situation. Then

$$p_k(t+dt) = [1-(2k+1)\,dt]p_k(t) + [k\,dt]p_{k-1}(t) + [(k+1)\,dt]p_{k+1}(t) \tag{5}$$

as may be seen by considering which states at time t could lead to state k at time $t + dt$ and using (4). Equation (5) provides the system of differential equations

$$\frac{dp_k(t)}{dt} = -(2k+1)p_k(t) + kp_{k-1}(t) + (k+1)p_{k+1}(t), \qquad k = 0, 1, 2, \cdots. \tag{6}$$

In terms of the generating function

$$P(x, t) = \sum_{k=0}^{\infty} p_k(t)x^k, \qquad 0 \leqq x \leqq 1, \tag{7}$$

we obtain from (16)

$$\frac{\partial P}{\partial t} = (1-x)^2\frac{\partial P}{\partial x} - (1-x)P. \tag{8}$$

This is a first-order partial differential equation, which can be handled by standard procedures to yield the general solution

$$P(x, t) = \frac{1}{1-x} f\left\{\frac{1-x}{1+(1-x)t}\right\}, \tag{9}$$

where f is an arbitrary function. The boundary condition comes from the initial situation

$$p_0(0) = 1, \qquad p_k(0) = 0, \qquad k > 0, \tag{10}$$

which is equivalent to

$$1 = P(x, 0) = \frac{1}{1-x} f(1-x). \tag{11}$$

Hence $f(y) = y$ for $0 \leqq y \leqq 1$; and (9) becomes

$$P(x, t) = \frac{1}{1+(1-x)t}. \tag{12}$$

By expanding (12) as a power series in x, we deduce

$$p_k(t) = \frac{t^k}{(1+t)^{k+1}}, \qquad k = 0, 1, 2, \cdots. \tag{13}$$

Equalities (12) and (13) lead to various conclusions, of which the following are typical. The rth factorial moment of the state number at time t is

$$E(k^{\{r\}}) = \left[\frac{\partial^r}{\partial x^r}\left\{\frac{1}{1+(1-x)t}\right\}\right]_{x=1} = r!\, t^r. \tag{14}$$

In particular, the expected state number is

$$E(k) = E(k^{\{1\}}) = t; \tag{15}$$

and the variance of the state number is

$$E(k^{\{2\}}) + E(k)[1 - E(k)] = t(t+1). \tag{16}$$

Since

$$\frac{p_{k+1}(t)}{p_k(t)} = \frac{t}{1+t} < 1, \tag{17}$$

the probability at any given time of occupying any given state is a decreasing function of the state number; and the most likely state is the ground state $k = 0$. If the process runs for a time duration T, the expected time spent in state k is

$$m_k(T) = \int_0^T p_k(t)\, dt. \tag{18}$$

The integral (18) can be evaluated directly from (13); but it is more convenient to use (12), as follows.

$$M(x, T) = \sum_{k=0}^{\infty} m_k(T) x^k = \int_0^T P(x, t)\, dt = \frac{\log[1+(1-x)T]}{1-x}. \tag{19}$$

The coefficient of x^k on the right of (19) yields

$$m_0(T) = \log(1 + T) \tag{20}$$

and

$$m_k(T) = \log(1 + T) - \sum_{r=1}^{k} \frac{T^r}{r(1 + T)^r}, \qquad k > 0. \tag{21}$$

Hence

$$\log(1 + T) - \sum_{r=1}^{k} r^{-1} \leqq m_k(T) \leqq \log(1 + T); \tag{22}$$

whence, for any fixed k,

$$m_k(T) \sim \log T \quad \text{as} \quad T \to \infty. \tag{23}$$

If the particle is known to have just arrived in some given state k, the expected time it will remain there before visiting some other state is $1/(2k + 1)$, by virtue of the second equation in (4). Since this quantity is finite whereas the right side of (23) tends to infinity as $T \to \infty$, we conclude that the state k is visited infinitely often when the process continues indefinitely; and hence every state is visited infinitely often.

Finally consider how things will appear to an observer who watches a fixed point on the line. In a short interval of time, of fixed length Δt and uniformly random onset, the conditional probability that the light particle will be observed to cross this point given that it has velocity v is $v\Delta t = (k + 1/2)\,\Delta t$. Hence the relative frequency of velocities of observed particles will be proportional to $(k + 1/2)p_k(t)$. Using (13) and summing over k to evaluate to constant of proportionality, we find that the relative frequencies are

$$f_k(t) = \frac{\left(k + \frac{1}{2}\right)t^k}{\left(\frac{1}{2} + t\right)\left(1 + t\right)^{k+1}}, \qquad k = 0, 1, \cdots. \tag{24}$$

The mode of this distribution occurs when k is close to $t + 1/2$. The mean is

$$2t + \frac{t}{2t + 1} \tag{25}$$

and the variance is

$$2t(t + 1) + \frac{1}{(2t + 1)^2}. \tag{26}$$

To see the asymptotic behavior of k for large t, we make the transformation $z = k/t$, which reduces (24) to the form

$$ze^{-z}\,dz \tag{27}$$

when $t \to \infty$.

It might be possible to extend the foregoing analysis in several directions. For instance, an isotropic random factor might be introduced into the right side of (1) to simulate collisions in three-dimensional space; and the analysis might be modified to allow the weightless particle to have some definite fraction of the weight of the heavy particles. But these extensions will not be pursued here.

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