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Irreversibility and Nonrecurrence

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Zermelo and Loschmidt pointed out that the equations of classical mechanics are recurrent and reversible, while those of macroscopic physics are nonrecurrent and irreversible. These observations cast doubt on the possibility of deriving the macroscopic equations from classical mechanics. Therefore an example is presented to show that nonrecurrent equations can be derived from recurrent ones, and another example to show that irreversible equations can be derived from reversible ones. The irreversible equation derived in the second example describes either decaying, growing, or undamped motions, depending upon the initial conditions. Thus the specification of initial conditions introduces the irreversibility. These demonstrations may help to clarify previous resolutions of the recurrence and reversibility paradoxes.

KEY WORDS: Irreversibility; nonrecurrence; Langevin equation.

1. INTRODUCTION

Attempts to derive equations governing macroscopic matter from those of classical mechanics for microscopic matter have raised two problems. First Loschmidt (1876) noted that the classical mechanical equations are reversible while the macroscopic equations are not. Then Zermelo (1896) observed that the motions of bounded classical mechanical systems are recurrent, while macroscopic motions are not. It is a paradox that irreversible equations should arise from reversible ones, and another paradox that nonrecurrent equations should follow from recurrent ones. These paradoxes have been resolved, but this fact is not generally realized because the resolutions are obscured by mathematical and physical complications.

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Our goal is to resolve the paradoxes clearly and simply, and to show where irreversibility is introduced. Since the paradoxes are essentially mathematical, we reformulate them as mathematical questions:

1. Can nonrecurrent equations be derived from recurrent equations?
2. Can irreversible equations be derived from reversible equations?

To answer the first question, various authors have shown that for certain classical N degree of freedom systems, the recurrence time tends to infinity with N. Therefore the recurrent equations of motion for these systems tend to nonrecurrent ones. However the limiting equations are still reversible.

To answer the second question one must consider systems with N tending to infinity, or with N infinite, to avoid recurrence. For certain such systems, a number of authors have derived equations for some degrees of freedom by eliminating or projecting out the other degrees of freedom. This projection method has yielded irreversible equations in which motions decay in time.

It has not been realized that exactly the same method applied to the same systems can also yield irreversible equations in which the motions *grow* in time. Whether the motions decay or grow or do neither depends upon the initial conditions of the system. Furthermore these conditions also determine the decay or growth rate.

This result leads to the conclusion that the symmetry between past and future, possessed by the original equations, is not broken by letting N become infinite nor by projecting out some degrees of freedom. It is broken by specifying a particular initial condition. This is understandable because the operations of taking the limit $N \to \infty$ and projecting out degrees of freedom both commute with time reversal, while specifying an initial condition does not.

Now we describe the contents of the rest of this paper. In Section 2 we apply the projection method to a particle attached to a spring and to an infinitely long string, which is a system with infinitely many degrees of freedom. We obtain an irreversible equation for the particle motion, in which the damping is either positive, negative, or zero depending upon the initial conditions.

In Section 3 we derive an equation for the density of N free particles moving around on a circle in the limit $N \to \infty$. This equation is nonrecurrent but reversible. In Section 4 we compare the density for N finite with that for N infinite. In Section 5 we present some concluding remarks and references to some of the relevant previous work.

2. A PARTICLE ON A STRING

To show how an irreversible equation can be derived from reversible ones, we consider an infinitely long string which performs small-amplitude transverse vibrations in the x, y plane about the x axis. We denote by $U(x, t)$ its displacement at position x and time t, and we write its equation of motion as

$$U_{tt} = c^2 U_{xx}, \qquad x \neq 0 \tag{1}$$

Here c is the speed of transverse waves. A particle of mass M is attached to the string at $x = 0$, and is also attached to a linear or nonlinear spring. We let $Z(t)$ be the displacement of the particle in the y direction, and $-F(Z)$ be the restoring force exerted on it by the spring. Then the equation of motion of the particle, and the condition of attachment to the string, are

$$MZ_{tt} + F(Z) = \sigma[U_x(0+, t) - U_x(0-, t)] \tag{2}$$

$$Z(t) = U(0, t) \tag{3}$$

In (2) σ denotes the tension in the string.

Lamb[1] considered this problem with $F(Z)$ linear in Z and with the string semi-infinite. He used it to explain why the field radiated by a damped oscillator increases with distance from the oscillator, but he did not consider irreversibility.

The equations (1)–(3) govern the motion of the system. They are reversible, as we can see from the fact that they involve only second derivatives with respect to t. Thus if $U(x, t)$, $Z(t)$ is a solution, so is the time-reversed motion $U(x, -t)$, $Z(-t)$.

A particular solution of (1) which satisfies (3) is the outgoing wave solution

$$U(x, t) = Z(t - |x|/c) \tag{4}$$

Upon using (4) to eliminate U from (2), we obtain the following equation for Z:

$$MZ_{tt} + \frac{2\sigma}{c} Z_t + F(Z) = 0 \tag{5}$$

This is the equation of a damped nonlinear oscillator with no external force. It is clearly irreversible because of the Z_t term, so we have shown that an irreversible equation can be derived exactly from reversible equations, answering question 2 affirmatively.

It is tempting to conclude that, because of radiation of waves along the string, the particle motion must be positively damped as it is in (5). This conclusion is incorrect, as we see by considering instead of (4) the incoming wave solution

$$U(x, t) = Z(t + |x|/c) \tag{6}$$

It also satisfies (1) and (3). When used in (2) it yields

$$MZ_{tt} - \frac{2\sigma}{c} Z_t + F(Z) = 0 \tag{7}$$

This equation for Z has negative damping. Energy is supplied to the particle by waves on the string traveling toward the particle.

The two solutions (4) and (6) for U differ in their initial values and initial velocities at $t=0$. Thus the sign of the damping coefficient in (5) or (7) is determined by the initial conditions of the string. We shall now show that even the magnitude of this coefficient is determined by those conditions.

Let us write the general solution of (1) satisfying (3) in the form

$$U(x, t) = \alpha Z(t - |x|/c) + (1-\alpha)\, Z(t + |x|/c) + u(x, t) \tag{8}$$

Here α is any real number and $u(x, t)$ is any solution of (1) which vanishes at $x=0$:

$$u_{tt} = c^2 u_{xx}, \qquad x \neq 0 \tag{9}$$

$$u(0, t) = 0 \tag{10}$$

Substitution of (8) into (2) yields

$$MZ_{tt} + (2\alpha - 1)\frac{2\sigma}{c} Z_t + F(Z) = f(t) \tag{11}$$

where

$$f(t) = \sigma[u_x(0+, t) - u_x(0-, t)] \tag{12}$$

We see that in the equation (11) for Z, the damping coefficient can have any real value, depending upon the choice of α. The choices $\alpha = 1$ and $\alpha = 0$ yield the values in (5) and (7), respectively. The choice $\alpha = 1/2$, corresponding to half incoming and half outgoing waves, yields the damping coefficient zero. Since the different solutions (8), which give rise to these choices, differ only in their initial conditions, it follows that the initial conditions play an essential role in determining the damping coefficient and the nature of the irreversibility.

3. PARTICLES ON A CIRCLE

To illustrate how recurrence can be eliminated, we shall consider N noninteracting particles, moving along the circumference of a circle. Let $\varphi_j(t)$ be the angular position of particle j at time t. We take the equations of motion to be

$$\frac{d^2\varphi_j}{dt^2}=0, \qquad j=1,..., N \tag{13}$$

These equations are obviously reversible. Their solution with initial position φ_j^0 and initial angular velocity ω_j is

$$\varphi_j(t)=\varphi_j^0+\omega_j t \tag{14}$$

To show that the motion is recurrent, we first suppose that for each j, $\omega_j/2\pi=p_j/q_j$, where p_j and q_j are integers. Thus we suppose that each $\omega_j/2\pi$ is a rational number. Then at the time $t_n^*=nq_1q_2\cdots q_N$, where n is an integer, it follows that $\omega_j t_n^*=2\pi np_jq_1\cdots q_{j-1}q_{j+1}\cdots q_N$, so $\omega_j t_n^*$ is an integer multiple of 2π. Then (14) shows that $\varphi_j(t_n^*)=\varphi_j^0 \bmod 2\pi$, so at t_n^* each particle has returned exactly to its initial position. Thus the motion is periodic with period t_1^*. When $\omega_j/2\pi$ is irrational, it can be approximated arbitrarily closely by a rational number if the denominator q is chosen large enough. From this it can be shown that for any set of ω_j there is also a sequence of times, tending to infinity, at which all the particles return arbitrarily close to their initial positions. Therefore the motion is called recurrent. Estimates of the way in which these recurrence times increase with N have been determined by Frisch,(2) Hemmer (see Ref. 3) and Wergeland.(3)

Next we introduce the angular velocity ω and the fractional number density $f_N(\varphi, \omega, t)$, defined by

$$f_N(\varphi, \omega, t)=\frac{1}{N}\sum_{j=1}^{N}\delta[\varphi_j(t)-\varphi]\,\delta[\omega_j-\omega] \tag{15}$$

By direct substitution, using the fact that $d\omega/dt=0$, we can verify that f_N satisfies the differential equation

$$\partial_t f_N+\omega\partial_\varphi f_N=0 \tag{16}$$

This equation is equivalent to the system (13), so its solutions are also reversible and recurrent.

We now assume that as N becomes infinite, f_N has a weak limit f:

$$\lim_{N\to\infty} f_N(\varphi, \omega, t)=f(\varphi, \omega, t) \tag{17}$$

Then it follows from (16), under some mild conditions, that f satisfies

$$\partial_t f + \omega \partial_\varphi f = 0 \tag{18}$$

Replacement of t and ω by $-t$ and $-\omega$ leaves (18) unchanged, so it is reversible. Its solution with initial condition $f(\varphi, \omega, 0) = f_0(\varphi, \omega)$ is

$$f(\varphi, \omega, t) = f_0(\varphi - \omega t, \omega) \tag{19}$$

We shall prove next that f is not recurrent by considering the angular number density $\rho(\varphi, t)$ defined by

$$\rho(\varphi, t) = \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} f(\varphi - 2\pi n, \omega, t)\, d\omega \tag{20}$$

By using (19) for f in (20) and then setting $x = \varphi - \omega t - 2\pi n$ we get

$$\begin{aligned} \rho(\varphi, t) &= \int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} f_0(\varphi - \omega t - 2\pi n, \omega)\, d\omega \\ &= -\int_{-\infty}^{\infty} \sum_{n=-\infty}^{\infty} f_0\left(x, \frac{\varphi - x - 2\pi n}{t}\right) \frac{dx}{t} \end{aligned} \tag{21}$$

As t becomes infinite, the last sum in (21) converges to a Riemann integral. If we write $dy = -2\pi/t$, we obtain from (21) and the fact that f_0 is normalized, the result

$$\lim_{t \to \pm\infty} \rho(\varphi, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_0(x, y)\, dy\, dx = \frac{1}{2\pi} \tag{22}$$

This shows that ρ converges to a limit as t becomes infinite, which cannot be the case if f is recurrent. Therefore f is nonrecurrent.

Frisch[4] has also shown that the density and other macroscopic quantities tend to limits as t tends to $+\infty$ and as t tends to $-\infty$, and that these limits are equal. His analysis is based upon the introduction of the probability distribution function of statistical mechanics, rather than on the limit $N \to \infty$ in the deterministic case considered above.

We have now shown in an example that by letting N become infinite, we obtain an equation which is nonrecurrent but still reversible. It was to avoid recurrence that we began with a system with infinitely many degrees of freedom in Section 2.

4. COMPARISON OF DENSITIES FOR N FINITE AND INFINITE

The angular number density $\rho_N(\varphi, t)$ for finite N is defined by (20) with f replaced by f_N. When (15) is used for f_N in (20) it yields

$$\rho_N(\varphi, t) = \frac{1}{N} \sum_{j=1}^{N} \sum_{n=-\infty}^{\infty} \delta(\varphi_j^0 + \omega_j t - \varphi - 2\pi n) \tag{23}$$

The particle motion for N finite is recurrent, so $\rho_N(\varphi, t)$ is recurrent, while $\rho(\varphi, t)$ is nonrecurrent. Therefore if ρ and ρ_N are equal or nearly equal at $t=0$, they cannot remain nearly equal indefinitely. After a finite time, which depends upon N, they must become very different. This is so because $\rho(\varphi, t)$ tends to a limit as t increases, while $\rho_N(\varphi, t)$ returns arbitrarily close to its initial value infinitely often. We shall now evaluate ρ and a smoothed version of ρ_N in a special case in order to compare them.

To calculate ρ_N, we set $N=2M+1$ and start with all particles at the origin, so $\varphi_j^0=0$ for all j. We take the initial angular velocities to be equally spaced with $\omega_j=j/(2M+1)$, $j=-M,..., M$. In addition we average ρ_N over an interval of length ε centered at φ, and call the smoothed density $\rho_{N,\varepsilon}(\varphi, t)$. Thus by using (23) and these initial conditions we get

$$\begin{aligned}\rho_{N,\varepsilon}(\varphi, t) &= \frac{1}{\varepsilon}\int_{-\varepsilon/2}^{\varepsilon/2} \rho(\varphi+\theta, t)\, d\theta \\ &= \frac{1}{(2M+1)\varepsilon}\sum_{j=-M}^{M}\sum_{n=-\infty}^{\infty}\int_{-\varepsilon/2}^{\varepsilon/2} \delta\left(\frac{jt}{2M+1}-\varphi-2\pi n-\theta\right) d\theta\end{aligned} \tag{24}$$

The last integral is zero unless n lies in the interval

$$\frac{1}{2\pi}\left(\frac{jt}{2M+1}-\varphi-\frac{\varepsilon}{2}\right)<n<\frac{1}{2\pi}\left(\frac{jt}{2M+1}-\varphi+\frac{\varepsilon}{2}\right) \tag{25}$$

When n does lie in this interval, the integral is unity. Therefore (24) can be rewritten

$$\begin{aligned}\rho_{N,\varepsilon}(\varphi, t) = \frac{1}{(2M+1)\varepsilon}\sum_{j=-M}^{M}&\left\{\left[\frac{1}{2\pi}\left(\frac{jt}{2M+1}-\varphi+\frac{\varepsilon}{2}\right)\right]\right. \\ &\left. -\left[\frac{1}{2\pi}\left(\frac{jt}{2M+1}-\varphi-\frac{\varepsilon}{2}\right)\right]\right\}\end{aligned} \tag{26}$$

Here $[x]$ denotes the integer part of x.

The corresponding density $\rho(\varphi, t)$ is given by (21) with

$$\begin{aligned} f_0(\varphi, \omega) &= \delta(\varphi), \qquad & -1/2<\omega<1/2 \\ &= 0, & |\omega|>1/2 \end{aligned} \tag{27}$$

It is also the limit of $\rho_{N,\varepsilon}(\varphi, t)$ as N tends to infinity and ε tends to zero. By calculating it either from (21) and (27), or from (26) as $N \to \infty$ and $\varepsilon \to 0$, we get

$$\rho(\varphi, t) = \rho_{\infty,0}(\varphi, t) = \frac{1}{t}\left\{\left[\frac{1}{2\pi}\left(\frac{t}{2} - \varphi\right)\right] + \left[\frac{1}{2\pi}\left(\frac{t}{2} + \varphi\right)\right]\right\} \tag{28}$$

Here also $[x]$ denotes the integer part of x.

For M finite, the $2M+1$ particles have angular velocities which are integer multiples of $1/(2M+1)$. Therefore their motion is periodic with period $(2M+1)\,2\pi$, so $\rho_N(\varphi, t)$ is periodic with this period. But $\rho(\varphi, t)$ given by (28) is neither periodic nor recurrent. In fact, as (22) shows, $\rho(\varphi, t)$ tends to $1/2\pi$ as t becomes infinite.

In Fig. 1 we show two periods of $\rho_{2M+1,\varepsilon}(\pi, t)$ for $\varepsilon = 0.1$ and $M = 500$. We see that small fluctuations have much smaller recurrence times than the period $(2M+1)\,2\pi \approx 6289$, which is the recurrence time of the largest fluctuations. In Figs. 2 and 3 we show $\rho(\pi, t)$ and $\rho_{2M+1,\varepsilon}(\pi, t)$ for $\varepsilon = 0.1$ with $M = 100$ in Fig. 2 and $M = 5000$ in Fig. 3. We see that the limit density $\rho(\pi, t)$ is a good approximation to the density with $2M+1 = 10\,001$ as far as the calculation extends, which is only to $t = 500$. The figures also show that $\rho(\pi, t)$ tends to $1/2\pi \approx 0.15$ as t becomes infinite.

From (24) or (26) we see that $\rho_{2M+1,\varepsilon}(\pi, t)$ is even in t and periodic with period $T = (2M+1)\,2\pi$. Therefore $\rho_{2M+1,\varepsilon}(\pi, T-t) = \rho_{2M+1,\varepsilon}(\pi, -t) = \rho_{2M+1,\varepsilon}(\pi, t)$. This shows that the graph of $\rho_{2M+1,\varepsilon}(\pi, t)$ in

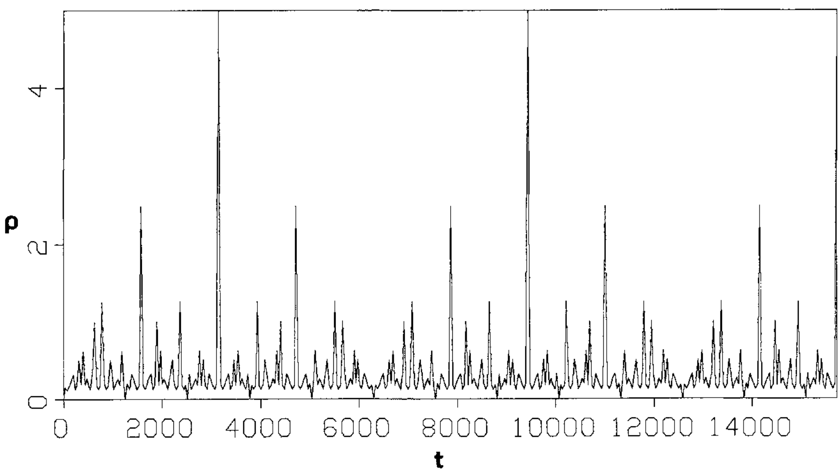

Fig. 1. Number density $\rho_{2M+1,\varepsilon}(\pi, t)$ versus time t for $M = 500$, $\varepsilon = 0.1$. Two complete periods are depicted. The period is $(2M+1)\,2\pi \approx 6289$.

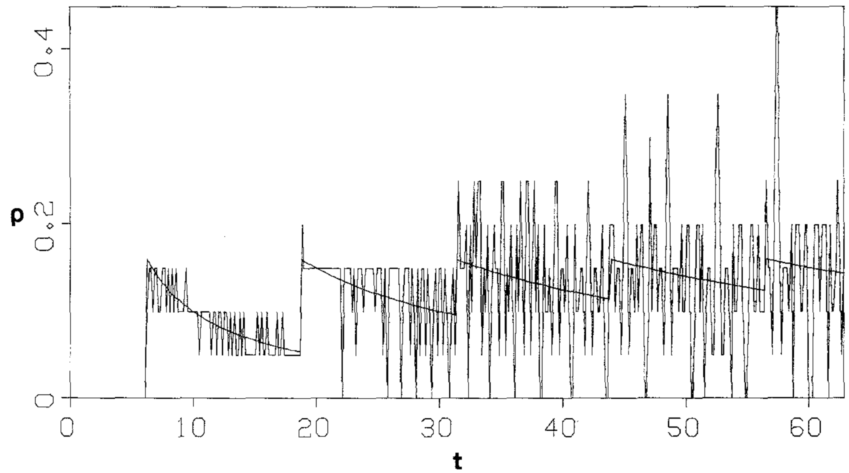

Fig. 2. Number densities $\rho_{2M+1,\varepsilon}(\pi, t)$ and $\rho(\pi, t)$ versus time t for $M=100$, $\varepsilon=0.1$. The period of $\rho_{201,0.1}(\pi, t)$ is approximately 1263. The limit density ρ has the graph with fewer jumps.

the interval $T-500<t<T$ is the same as that for $-500<t<0$, which is the mirror image of that for $0<t<500$. For $M=5000$ and $\varepsilon=0.1$ it is the same as the graph in Fig. 3 with the abscissa denoting $T-t$. The graph shows that $\rho_{2M+1,\varepsilon}(\pi, t)$ hovers around the value $1/2\pi$ at $T-t=500$ and then as $T-t$ tends to zero it oscillates with increasing downward jumps

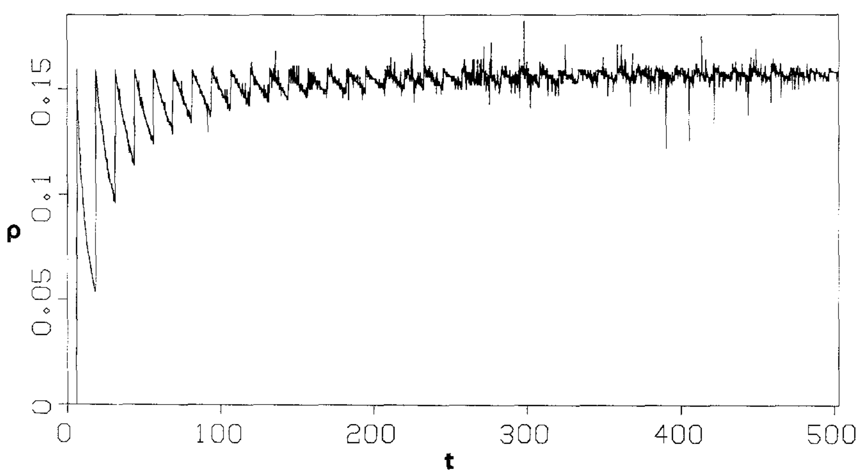

Fig. 3. Number densities $\rho_{2M+1,\varepsilon}(\pi, t)$ and $\rho(\pi, t)$ versus time t for $M=5000$, $\varepsilon=0.1$. The period of $\rho_{10\,001,0.1}(\pi, t)$ is about 62 382. The graph of $\rho(\pi, t)$ is hidden by the curve for $\rho_{10\,001,0.1}(\pi, t)$ which oscillates over it. With the axis denoting $62\,382-t$, the graph also represents $\rho_{10\,001,0.1}(\pi, t)$ for t near the end of a period.

until it reaches zero near the end of the first period. The graph of $\rho(\pi, t)$, which is not shown in Fig. 3 for this range of t, is practically constant at the value $1/2\pi$. Thus the two functions differ greatly in this range of t.

5. CONCLUDING REMARKS

1. When the string is initially in thermal equilibrium at temperature T, the force $f(t)$ in (11) is a Gaussian random function with mean zero and correlation function $\langle f(t) f(t') \rangle = 2kT\sigma^2 c^{-1} \delta(t-t')$, where k is Boltzmann's constant. This follows from the work of Keller,[5] and was also shown by Lewis and Thomas.[6] Then with $\alpha = 1$, (11) is just the Langevin equation. The relation between the damping constant in it and the correlation function yields the fluctuation–dissipation theorem. An earlier derivation was given by Zwanzig.[7]

2. The particle–string model illustrates the projection method.[8–11] This method concerns a system with macroscopic coordinates $Z(t)$ and internal or heat bath coordinates $U(t)$, satisfying equations of the form

$$Z_t = F(Z, U), \qquad U_t = G(Z, U) \tag{29}$$

The second equation is solved for $U(t)$ in terms of $Z(t)$ and substituted into the first equation to yield an equation for $Z(t)$ alone. When the system is infinite dimensional this equation may be irreversible even if the original system is reversible. Whether its solutions decay or grow in time depends upon the initial condition $U(0)$, as is shown by the example in Section 2.

3. Lebowitz and Spohn (Ref. 12, p. 597), in studying self-diffusion of colored particles, asked "For which initial dynamical states is the time evolution of the color density well approximated by a kinetic equation?" They realized that an irreversible diffusion equation could be derived only for certain initial conditions, in agreement with the result in Section 2.

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