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A generalisation of the Ehrenfests' wind–tree model

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Abstract We discuss a simple model for the relaxation of two interacting dynamical systems, based on the Ehrenfests' wind–tree model. It is still exactly solvable if Boltzmann's *Stosszahlansatz* is assumed to hold.

Samenvatting We bespreken een eenvoudig model voor de relaxatie van twee dynamische systemen met interactie, gebaseerd op het wind–bos model van P en T Ehrenfest. Onder aanname van de geldigheid van de *Stosszahlansatz* is ons model nog steeds exact oplosbaar.

1 Introduction

In many instances simple models offer great help in understanding the basic phenomena of physics. In the following we shall describe a generalisation of the Ehrenfests' wind–tree model in order to study the approach to equilibrium of two interacting dynamical systems. This generalisation exhibits some interesting features, which are not present in the original model.

The wind–tree model was introduced by Ehrenfest and Ehrenfest (1911) in their famous review article on the foundations of statistical mechanics. Its main objective was to clarify which assumptions, made in the derivation of the Boltzmann equation, introduce the irreversibility in this equation. In the model a gas of 'wind particles' moves in between a random array of square 'trees'. The trees are all fixed with the same orientation, whereas the wind particles move with constant speed v in the four directions parallel to the diagonals (see figure 1). There is no interaction between the wind particles, so that the direction in which they move is only changed by collisions with the trees.

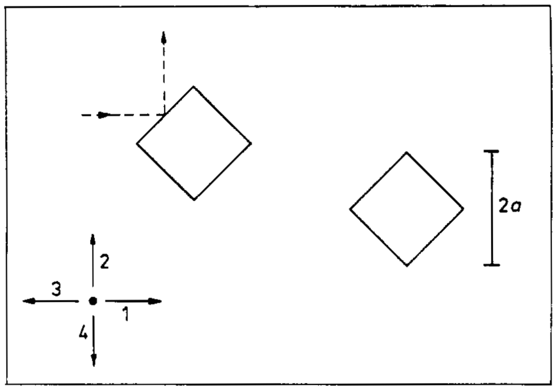

Figure 1 Square 'trees' of the Ehrenfests' model, which scatter 'wind' particles (broken line).

The rate equation for N_i, the average number of wind particles moving in the ith direction, is†

$$\frac{dN_i}{dt} = -\frac{2avZ}{\Omega}(N_i - \tfrac{1}{2}N_{i+1} - \tfrac{1}{2}N_{i-1}), \qquad (1)$$

where $2a$ is the length of the diagonals of the trees, Z is the number of trees, and Ω is the free area between the trees‡.

One arrives at equation (1) only if all correlations and memory effects are neglected: it is as if after each collision the wind particles are again randomly distributed, the only restriction being that each wind particle continues to move in the same direction as just before the redistribution. This of course amounts to the *Stosszahlansatz*; it limits the validity of equation (1) to the regime where the total area occupied by the trees is small compared with Ω, that is

$$2a^2Z \ll \Omega. \qquad (2)$$

Only then will the effects of 'ring collisions' and possible overlap of trees§ be negligible. The *Stosszahlansatz* accounts for the irreversible approach

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† The indices are used modulo 4. Hence $N_5 \equiv N_1$ and $N_0 \equiv N_4$ if $i = 4$ and 1 respectively in equation (1).

‡ The quantity $2av\,dt$ is the collision cylinder for a particle moving in a particular direction. Therefore the probability of hitting a tree in a time interval dt will be $2av\,dt/\Omega$. When there are Z trees and N_i particles moving in the ith direction, the first term in brackets is due to the loss of these particles through scattering, while the other two terms are due to the gain of particles moving in this direction.

§ These effects become increasingly important at higher densities for they cause the breakdown of a density expansion for the diffusion coefficient. For a more elaborate discussion of this point within the context of an Ehrenfest wind–tree model we refer to Hauge and Cohen (1969).

to equilibrium†.

Although equation (1) may be solved easily, the approach to the equilibrium state where

$$N_1^{eq}=N_2^{eq}=N_3^{eq}=N_4^{eq}=\tfrac{1}{4}N, \qquad (3)$$

N being the total number of wind particles, may also be derived by introducing Boltzmann's H function. This function is defined here by

$$H_w=\sum_{i=1}^{4} N_i \ln N_i. \qquad (4)$$

With the aid of equation (1) and the inequality

$$(x-y)\ln(x/y)\geqslant 0 \qquad (x, y>0) \qquad (5)$$

it is straightforward to show that

$$dH_w/dt\leqslant 0, \qquad (6)$$

where the equality sign holds in the equilibrium state. Thus the approach to equilibrium is established without the need to solve equation (1) explicitly.

The generalisation of the model to be discussed leads to the following new features:

(i) The relaxation depends explicitly on the initial conditions. For instance, if special initial conditions are chosen, the behaviour of some of the N_i is governed by a Gaussian exponential.

(ii) Contrary to what one finds in the original Ehrenfest model, the N_i may approach their equilibrium values non-monotonically.

(iii) In the H function the inclusion of a non-trivial term for the trees is required.

2 The generalised model

We consider a generalisation of the wind–tree model in which there are, besides the trees of the usual Ehrenfest model (which we call trees of type I), trees that are rotated through 45° (trees of type II; see figure 2). Thus trees of type I scatter wind particles from the direction i into perpendicular directions $i+1$ and $i-1$ (modulo 4) and hence give rise to an equilibration of wind particles in all directions. On the other hand, trees of type II scatter them into the opposite direction $i+2$ and tend to equilibrate only the directions 1 and 3, as well as 2 and 4, separately. Finally we endow the trees with a simple dynamical rule: each tree rotates through 45° immediately after it has been struck by a wind particle. Consequently a tree of type I transforms into a tree of type II and vice versa.

To start our analysis, we notice that the equilibrium values for the average number of wind particles moving in each direction will again be given by equation (3). This follows from symmetry considerations and the principle of detailed balance. The

†The Ehrenfests (1911, note 62) point out that the *Stosszahlansatz* cannot hold for both the direct and the inverse collisions.

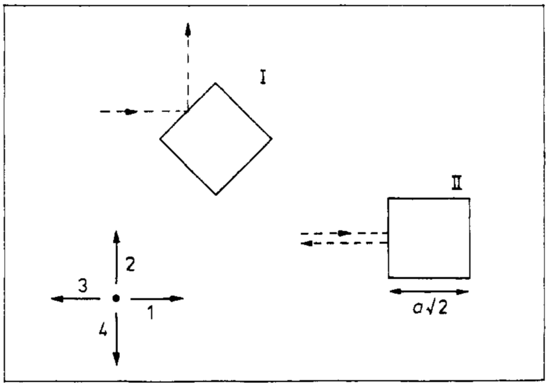

Figure 2 The two types of 'trees' of the generalised model, which scatter wind particles differently.

average numbers of trees of type I and type II, Z_I and Z_{II} respectively, are also determined in equilibrium by the principle of detailed balance. Taking into account that the scattering cross section of trees of type II is smaller than that of trees of type I by a factor $\sqrt{2}$, we find

$$Z_{II}^{eq}/Z_I^{eq}=\sqrt{2}. \qquad (7)$$

The rate equation for the wind particles becomes (cf equation (1))

$$\frac{dN_i}{dt}=\frac{Z_I}{\Delta}(-N_i+\tfrac{1}{2}N_{i+1}+\tfrac{1}{2}N_{i-1})+\frac{Z_{II}}{\sqrt{2}\Delta}(N_{i+2}-N_i), \qquad (8)$$

with

$$\Delta=\Omega/2av. \qquad (9)$$

Notice that as Δ is the average time after which one particular wind particle strikes one particular tree of type I, Z_I/Δ and $Z_{II}/\sqrt{2}\Delta$ are the collision frequencies of that wind particle on trees of type I and II respectively.

Since the rotation of a tree takes place irrespective of the direction in which the colliding wind particle moves, the rate equation for the trees depends only on the total number of wind particles N. Because this number is conserved, as is the total number of trees Z, the rate equation for the trees becomes linear:

$$\frac{dZ_I}{dt}=-\frac{N}{\Delta}Z_I+\frac{N}{\sqrt{2}\Delta}Z_{II}, \qquad (10)$$

$$Z_I+Z_{II}=Z. \qquad (11)$$

These last equations immediately yield

$$Z_I(t)=Z_I^{eq}+(Z_I(0)-Z_I^{eq})\exp(-t/T), \qquad (12)$$

with

$$T = \Delta/(1+\tfrac{1}{2}\sqrt{2})N, \tag{13}$$

$$Z_{\rm I}^{\rm eq} = Z/(1+\sqrt{2}). \tag{14}$$

Indeed $Z_{\rm I}$ approaches the equilibrium value given by detailed balance (equation (7)) with a relaxation time proportional to Δ divided by N; this ratio is essentially the average time between two collisions on a tree. For convenience, from now on we will choose T as our unit of time.

The solution (12)–(14) can be substituted into equation (8), which can then be solved as well. This leads to

$$N_i(t) = \tfrac{1}{4}N + \tfrac{1}{2}\alpha_i \exp(-G(t)) + \tfrac{1}{2}\beta_i \exp(-H(t)), \tag{15}$$

with

$$G(t) = (3\sqrt{2}-4)\frac{Z}{N}\left(3t - \frac{Z_{\rm I}(0)-Z_{\rm I}^{\rm eq}}{Z}[1-\exp(-t)]\right), \tag{16}$$

$$H(t) = (6\sqrt{2}-8)\frac{Z}{N}\left(t + \frac{Z_{\rm I}(0)-Z_{\rm I}^{\rm eq}}{Z_{\rm I}^{\rm eq}}[1-\exp(-t)]\right). \tag{17}$$

Here the constants α_i and β_i are determined by the initial conditions:

$$\alpha_i = N_i(0) - N_{i+2}(0), \tag{18}$$

$$\beta_i = N_i(0) + N_{i+2}(0) - \tfrac{1}{2}N. \tag{19}$$

From equations (15)–(17) it follows that the rate of relaxation of the wind particles towards equilibrium depends on the initial distribution of the trees, as well as on the density of the gas of wind particles relative to the trees, N/Z.

We will now discuss the properties of the solution, described by equations (15)–(19). One can distinguish two regimes: the dilute gas regime, when $N/Z \ll 1$; and the dense gas regime, $N/Z \gg 1$. In the dilute gas approximation the wind particles have a relaxation time much shorter than that of the trees, because each wind particle has already been scattered often before an appreciable number of trees is hit. In this case one may take $t \ll 1$ in studying the relaxation of the wind particles (remember that we measure time in units of the relaxation time T of the trees). Hence (using equation (14))

$$G(t) \approx (3\sqrt{2}-4)\frac{Z}{N}\left(2+\sqrt{2}-\frac{Z_{\rm I}(0)}{Z}\right)t \equiv \frac{t}{\tau_1}, \qquad t \ll 1, \tag{20}$$

$$H(t) \approx (6\sqrt{2}-8)\frac{Z}{N}\frac{Z_{\rm I}(0)}{Z_{\rm I}^{\rm eq}}\,t \equiv \frac{t}{\tau_2}, \qquad t \ll 1. \tag{21}$$

This leads to the usual decay law for the $N_i(t)$, a linear combination of exponentials. The leading relaxation time is determined by the value of $Z_{\rm I}(0)$:

$$\tau_1 \lesseqgtr \tau_2 \leftrightarrow Z_{\rm I}(0) \lesseqgtr \sqrt{2}Z_{\rm I}^{\rm eq}. \tag{22}$$

An exception occurs when $Z_{\rm I}(0)=0$. In this case the linear approximation (21) for $H(t)$ breaks down, and one finds a leading t^2 term in $H(t)$:

$$H(t) \approx (3\sqrt{2}-4)\frac{Z}{N}t^2 \equiv \gamma t^2, \qquad t \ll 1. \tag{23}$$

If one has, for example,

$$N_1(0) = N, \qquad N_2(0) = N_3(0) = N_4(0) = 0, \tag{24}$$

one finds a Gaussian time dependence for N_2 and N_4:

$$N_2(t) = N_4(t) = \tfrac{1}{4}N[1-\exp(-\gamma t^2)]. \tag{25}$$

The reason for this is that initially no wind particles are scattered into the directions 2 and 4 if all trees are of type II.

The dense gas approximation, on the other hand, is characterised by the relatively slow approach to equilibrium of the wind particles. In this case they move after a small transient time of order T between trees that have reached their equilibrium distribution. We then find (take $t \gg 1$ in equations (16) and (17))

$$G(t) \approx (3\sqrt{2}-4)\frac{Z}{N}\left(-\frac{Z_{\rm I}(0)-Z_{\rm I}^{\rm eq}}{Z}+3t\right) \equiv C_1 + \frac{t}{\tau_1}, \qquad t \gg 1, \tag{26}$$

$$H(t) \approx (6\sqrt{2}-8)\frac{Z}{N}\left(\frac{Z_{\rm I}(0)-Z_{\rm I}^{\rm eq}}{Z_{\rm I}^{\rm eq}}+t\right) \equiv C_2 + \frac{t}{\tau_2}, \qquad t \gg 1. \tag{27}$$

The presence of the constant terms C_1 and C_2, which rescale α_i and β_i by factors $\exp(-C_1)$ and $\exp(-C_2)$ respectively†, is the only reminder of this small transient regime. The relaxation times now have a fixed ratio

$$\tau_1 = \tfrac{2}{3}\tau_2. \tag{28}$$

An interesting property of the solution (15)–(19) is that it allows for non-monotonic relaxation. Consider, for example, the case described by the initial conditions (24). Substitution into equations (15)–(19) leads in particular to

$$N_3(t) = \tfrac{1}{4}N - \tfrac{1}{2}N\exp(-G(t)) + \tfrac{1}{4}N\exp(-H(t)). \tag{29}$$

† Notice that the qualitative behaviour of C_1 and C_2 as a function of the initial conditions may also be understood easily. As C_1 rescales $\alpha_i = N_i(0) - N_{i+2}(0)$, $\exp(-C_1)$ should be smaller, the larger the initial fraction of type II trees was (for these trees in particular equilibrate N_i and N_{i+2}). On the other hand, $\beta_i = N_i + N_{i+2} - \tfrac{1}{2}N$ will be reduced the more, the larger the initial fraction of type I trees was. Equations (26) and (27) agree with this qualitative picture. A similar explanation may be given for the qualitative behaviour in the other regime, as expressed by equations (20)–(22).

Although initially N_3 is equal to zero, it can exceed its equilibrium value according to equation (29) if

$$G(t) - H(t) > \ln 2. \qquad (30)$$

Using the explicit expressions (16) and (17) for G and H, it is straightforward to show that this condition is always satisfied for large times, irrespective of the initial distribution of the trees. This behaviour is exemplified for the case $N/Z = 1$ in figure 3. We emphasise that this 'overshoot effect' can exist even when the trees are not allowed to rotate but have a fixed distribution. Thus this effect can arise in linear Ehrenfest models†.

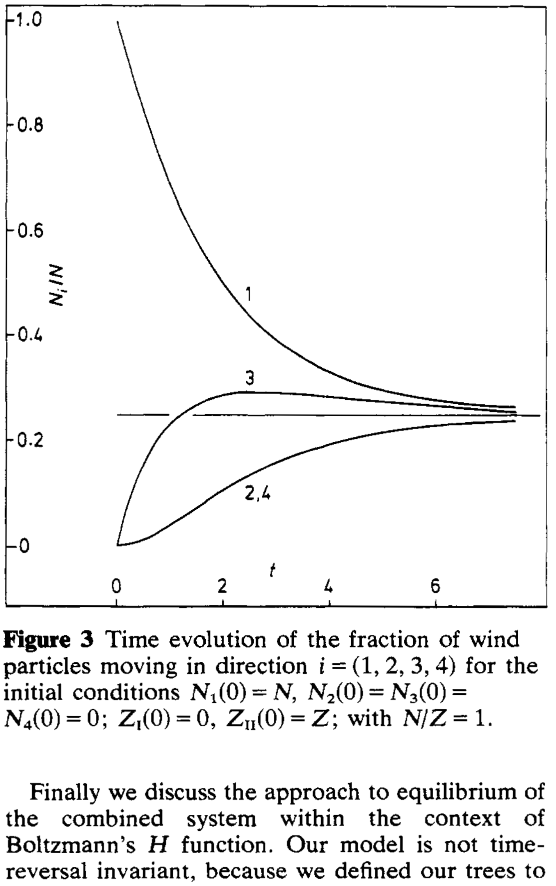

Figure 3 Time evolution of the fraction of wind particles moving in direction $i = (1, 2, 3, 4)$ for the initial conditions $N_1(0) = N$, $N_2(0) = N_3(0) = N_4(0) = 0$; $Z_I(0) = 0$, $Z_{II}(0) = Z$; with $N/Z = 1$.

Finally we discuss the approach to equilibrium of the combined system within the context of Boltzmann's H function. Our model is not time-reversal invariant, because we defined our trees to rotate *after* each collision. This leads to a modification in the definition of H. The H function is an additive quantity and can be written as

$$H = H_w + H_t. \qquad (31)$$

† Non-monotonic (that is, oscillatory) behaviour was found by Cohen (1979) in an Ehrenfest model with isosceles triangles. Overshoot effects were recently observed in numerical and analytical solutions of the non-linear Boltzmann equation (see e.g. Tjon 1979, Ernst 1980). However, one of the most interesting results of these calculations, namely that the overpopulation decays non-exponentially, can of course not be explained by quasi-linear models.

For H_w, which is defined in equation (4), the inequality (6) can, with the aid of equation (8), still be shown to hold. H_t is the contribution of the trees. The non-monotonic decrease of H is now established if

$$\mathrm{d}H_t/\mathrm{d}t \leqslant 0. \qquad (32)$$

The following form turns out to be appropriate:

$$H_t = Z_I \ln(\sqrt{2} Z_I) + Z_{II} \ln Z_{II}. \qquad (33)$$

Indeed, with the aid of equations (10), (11) and (15) we find

$$\frac{\mathrm{d}H_t}{\mathrm{d}t} = -\frac{N}{\sqrt{2}\Delta}(Z_I\sqrt{2} - Z_{II}) \ln\left(\frac{Z_I\sqrt{2}}{Z_{II}}\right) \leqslant 0. \qquad (34)$$

The presence of the factor $\sqrt{2}$ in the definition (33) is due to the different scattering cross sections of the two types of trees, and reflects the violation of time-reversal invariance.

3 Concluding remarks

Finally, we comment on the possible relevance of the model. It illustrates nicely how relaxation phenomena may depend on the initial conditions. However, it does not possess time-reversal invariance, as it is not a purely mechanical model. Therefore it seems more fit to describe phenomena such as chemical reactions.

Of course one can generalise the model still further in several ways. However, a few simple extensions we investigated did not lead to qualitatively different results.

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