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1990 J. Phys. A: Math. Gen. 23 1671

(http://iopscience.iop.org/0305-4470/23/10/010)

J. Phys. A: Math. Gen. **23** (1990) 1671-1687. Printed in the UK

A cellular automata model of large-scale moving objects

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Received 17 July 1989, in final form 12 December 1989

Abstract. We propose a reversible and local rule that allows large-scale objects called 'strings' to move with adjustable speed and energy in a three-dimensional space. We show that the motion of these strings is governed by discrete Hamiltonian equations and mediated by one longitudinal and two transverse sound waves that propagate along the string. This rule is a first attempt to model a solid body with a cellular automaton. It also provides interesting possibilities for simulating new physical situations.

1. Introduction

In the past few years cellular automata (CA) have received a great deal of attention, due in part to their ability to model various physical situations. It turns out that, in many of their recent applications (hydrodynamics [1-3], diffusion processes [4] or chemical reactions [5]), CA models deal with point-like particles that evolve on a lattice with very short-range interactions.

Although many interesting problems involving point-like particles are still to be investigated, CA should be able to model more complex objects, in order to extend their range of applicability. For instance, one may want to model molecules, which contain just a few bounded particles, or solid bodies, which are objects composed of many constituent particles and which have a coherent structure over large distances. To devise CA models that capture the properties of such physical systems turns out to be a very difficult task. Nevertheless, as a first step in this direction, we propose a simple time-reversible model that already contains some of the desired features, namely (*a*) to deal with large-scale objects (i.e. objects whose size is greater than range of the CA rule) which can move and interact with their surroundings, (*b*) to allow these objects to have adjustable mass, energy and momentum, and (*c*) that these objects maintain their size and their integrity during the evolution: deformations are allowed (these objects are not rigid), but the particles composing them should not spread out in the entire space.

The way we will define energy and momentum may be a matter of physical interpretation. For instance, it is very common to use a CA rule to describe a system of classical particles on a lattice and, as a result, to obtain a model of a fully discrete molecular dynamics. In these cases, an interpretation in terms of classical mechanics seems natural. But, on the automaton, the particles are not really moving from one site to another. In fact, it is only the state of the sites which are modified during time, without any transport of matter. Accordingly, CA should be more appropriate to model the propagation of a 'vacuum excitation' in some discrete field theory. In this case, a

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different physical interpretation may be required. However, we shall not consider this last approach because there is no evidence that our model reflects such a physical reality.

In the next section, we discuss in detail a CA rule recently studied by the author [6], as well as some of its extensions. An early version of this rule has been proposed by Margolus [7], and some of its abilities to model waves have been investigated by Hrgovčić [8]. The rule we will discuss in this paper models large-scale one-dimensional objects called 'strings' which can move in a one-, two- or three-dimensional space and which fulfil the conditions (*a*), (*b*) and (*c*). We will give some examples and describe some mechanisms that allow for limited interactions between two strings, or between strings and point-like particles.

Then we will show in section 3 that the rule which governs the evolution of our strings can be derived from discrete-time Hamiltonian equations. This approach provides a natural framework to define the physical quantities associated with the model and to discuss their conservation laws. Due to the breaking of continuous time translation invariance, we obtain a modified expression of the energy, which turns out to be conserved only for harmonic potentials.

Finally, in section 4, we discuss how sound waves are propagated through the string. Perfect transmission characterises the propagation inside the string while total reflection takes place at the end points. In spite of the discrete aspect of space and time, our rule can describe the propagation of any one-dimensional wave $\phi(i, t) = f(i-t)+g(i+t)$.

The aim of this paper is to present the basic principles that govern the dynamics of our string model. Applications to physical problems are proposed in section 5 and will be the subject of a subsequent paper in which numerical simulations will be considered.

2. A cellular automata rule for large-scale moving objects

Our strings are one-dimensional objects that can be thought of as chains of masses linked by springs.

More precisely, a string is composed of two kinds of particles, say the white ones and the black ones, which alternate along a polygonal line in a three-dimensional cubic lattice. The end points can be either colour.

In order to have a simple implementation of the rule, the string should not fold over onto itself. Therefore, we shall give an orientation to the string by imposing, in the initial configuration, that consecutive particles occupy positions with an increasing x coordinate. This choice is obviously arbitrary, and one can also choose the orientation along the y and z axes.

2.1. The rule

The time evolution has two phases. First, the black particles are held fixed and the white ones move according to the following prescription, applied independently for the x, y and z coordinates: the new configuration of the string is obtained by interchanging the spacings that separate the white particles from their two adjacent stationary black neighbours. In other words, the motion of a white particle consists of a reflection with respect to the centre of mass of its two black neighbour particles. More precisely, if $\boldsymbol{q}(t)$ is the position of a white particle on the lattice, and $\boldsymbol{q}_+$ and $\boldsymbol{q}_-$ are the positions

of the right and left adjacent black particles ('right' and 'left' are defined according to the direction of the x axis), then the new position $\boldsymbol{q}(t+1)$ of the white particle is given by

$$\boldsymbol{q}(t+1) = \boldsymbol{q}_+ + \boldsymbol{q}_- - \boldsymbol{q}(t). \tag{2.1}$$

Of course, this rule is only valid for a particle inside the string, which has exactly two neighbours. For the end points, the reflection is performed with respect to $\boldsymbol{q}_\pm \mp \boldsymbol{a}$, where $\boldsymbol{a}$ is a constant vector that represents the 'spring' linking the particles of the string together. According to the above convention of sign, the x component of $\boldsymbol{a}$ should be positive. Furthermore, to prevent the particles from moving off the lattice, $\boldsymbol{a}$ has to be integer or half-integer.

Thus, if the left end of the string is a white particle located at $\boldsymbol{q}(t)$, its new position will be

$$\boldsymbol{q}(t+1) = 2(\boldsymbol{q}_+ - \boldsymbol{a}) - \boldsymbol{q}(t) \tag{2.2}$$

and, similarly, if it is the right end, its new position will be

$$\boldsymbol{q}(t+1) = 2(\boldsymbol{q}_- + \boldsymbol{a}) - \boldsymbol{q}(t) \tag{2.3}$$

where $\boldsymbol{q}_+$ and $\boldsymbol{q}_-$ refer, respectively, to the positions of the particles next to the left end point and next to the right end point.

These two kinds of motion are illustrated in figure 1, for the two-dimensional case with $\boldsymbol{a} = (\frac{3}{2}, 0)$.

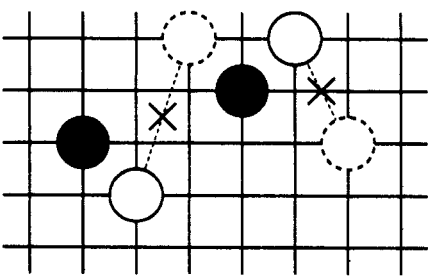

Figure 1. The string rule: during the first phase, the black particles are stationary. The internal white particle moves according to an inversion with respect to the centre of mass (denoted by the left cross) of its two surrounding neighbours. The end particle performs the reflection with respect to a point (the right cross) obtained by adding the vector $\boldsymbol{a}$ to the position of its nearest black neighbour (here, $\boldsymbol{a} = (\frac{3}{2}, 0)$). The broken particles indicate the new positions reached by the white particles during this time step.

The second phase of the rule is then to keep the white particles stationary, and to repeat the first phase with the black ones. The alternation of the movements of the black and white particles results in an overall motion of the string, as shown in figures 2 and 3.

As suggested by figure 2, and due to the fact that we chose the particles of the string to have increasing x coordinates, we call the motion along the x axis longitudinal, and the motions along the y and z axes transverse.

2.2. Mass, momentum and energy

Mass, momentum and energy can be associated with the strings in a simple way. These quantities turn out to be adjustable for a given string, and are conserved during the

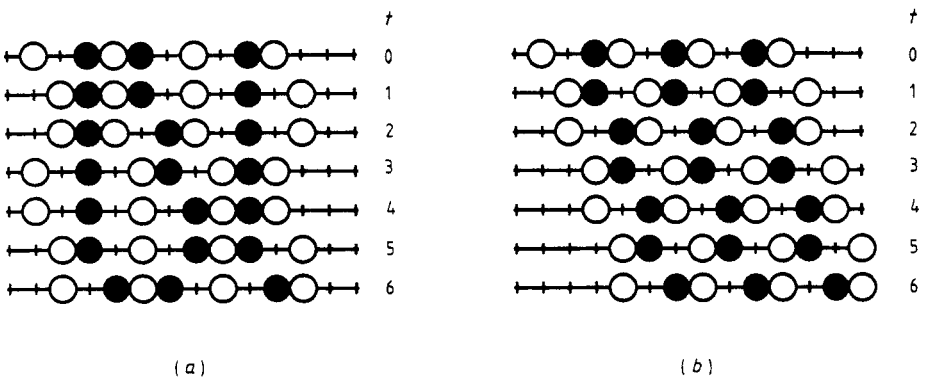

Figure 2. Typical motions of two longitudinal strings. The first one (*a*) needs exactly six time steps to cycle back to its initial configuration. Meanwhile, it has travelled one lattice spacing. Therefore, its speed is $\frac{1}{6}$. Similarly, the second string (*b*) has a cycle of two time steps, and its speed is $\frac{1}{2}$.

evolution. This point will be proven in the next section on the basis of a discrete Hamiltonian formalism.

In fact, we will show that the energy of a string is given by

$$E=\frac{1}{2}\sum_{i=1}^{N-1}[(x_{i+1}-x_i-a_x)^2+(y_{i+1}-y_i-a_y)^2+(z_{i+1}-z_i-a_z)^2] \tag{2.4}$$

where the index i labels the N particles composing the string, while x, y and z stand for their coordinates.

Moreover, the total momentum of a string is

$$\boldsymbol{P}=\tfrac{1}{2}\boldsymbol{v}_1+\sum_{i=2}^{N-1}\boldsymbol{v}_i+\tfrac{1}{2}\boldsymbol{v}_N \tag{2.5}$$

where $\boldsymbol{v}_i$ is the speed of the ith particle, i.e. the distance it will travel during the next time step. Relation (2.5) suggests that the total mass of a string should be $N-1$: $\frac{1}{2}$ for the end points and 1 for the internal particles.

From equations (2.4) and (2.5), it appears that the energy and momentum can indeed be adjusted by properly choosing the initial configuration of the string. The question is then to find the possible values of E and $\boldsymbol{P}$ a string can have, for a given length (or mass). As stated above, our evolution rule is valid for any set of separations between the particles. In practice, however, this is not true: the range of a CA rule is finite by definition and this constraint restricts the maximum values of the energy and momentum. In order to move, a particle must be able to see its two nearest neighbours. Due to the implicit finite range of the rule, one should impose

$$d_{\min}\leqslant w_{i+1}-w_i\leqslant d_{\max} \tag{2.6}$$

where w_i stands for x_i, y_i or z_i. Note that $d_{\min}$ and $d_{\max}$ may be different for each of the three spatial directions.

A natural choice would be $d_{\min}=-d_{\max}$. However, in order to preserve the orientation of the string and to prevent two particles occupying the same site or the string overlapping itself, we have to take $d_{\min}\geqslant 1$ for the longitudinal x motion.

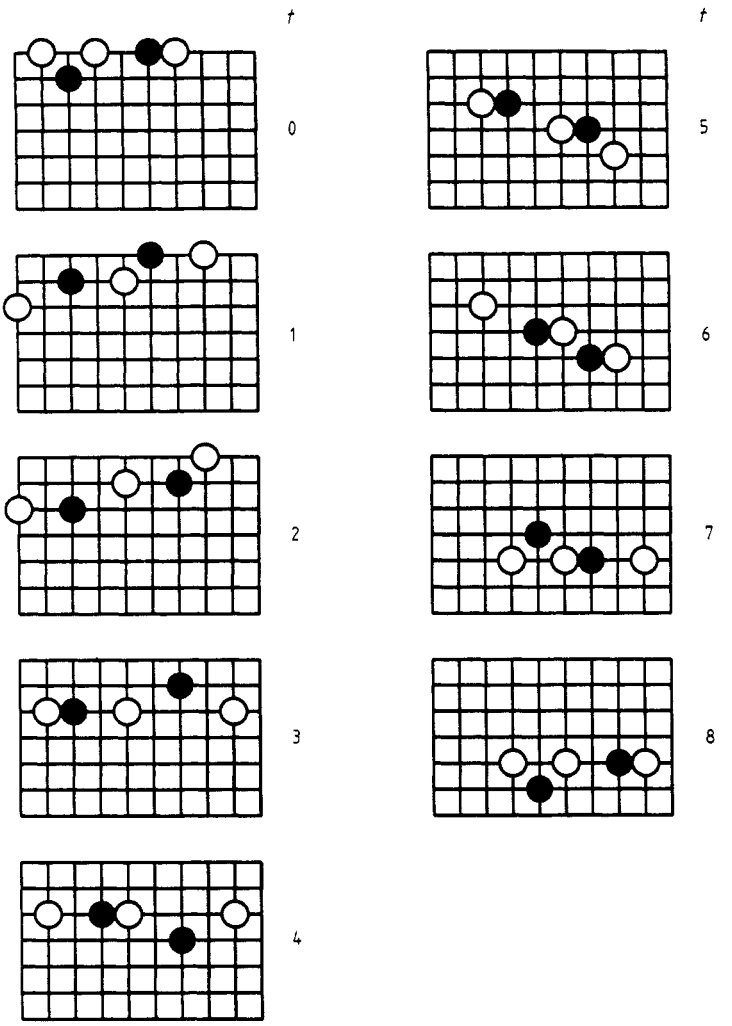

Figure 3. Motion of a string due to one longitudinal and one transverse sound wave. The same portion of the lattice is shown during the eight time steps that constitute the complete cycle. The speed of this string is $V_{CM} = (\frac{1}{4}; -\frac{1}{2})$, its mass is $M = 4$, its momentum is $P = (1; -2)$ and its energy is $E = 1$ ($a = (\frac{3}{2}; 0)$).

It is easy to check that the condition (2.6) remains valid during the evolution when considering an internal particle. Indeed, the rule consists of interchanging the spacings that separate the particle from its left and right neighbours. On the other hand, this property requires the proper choice of a for the terminal particles. For instance, let us consider the case of the first particle of the string, whose position is q_1. According to (2.2), its new position q_1' obeys

$$q_2 - q_1' = q_1 - q_2 + 2a.$$

Then, assuming that (2.6) holds for $q_2 - q_1$, we have

$$-d_{\max} + 2a_w \leqslant w_2 - w_1' \leqslant -d_{\min} + 2a_w.$$

In order to fulfil (2.6) again for the new position, a_w should be equal to

$$a_w = \tfrac{1}{2}(d_{\min} + d_{\max}). \tag{2.7}$$

For the transverse y and z motions, we will choose

$$d_{\min} = -d_{\max}.$$

This yields

$$a_y = a_z = 0.$$

The motion shown in figure 3 corresponds to a situation where $d_{\min} = 1$, $d_{\max} = 2$ for the longitudinal motion (i.e. $a_x = \frac{3}{2}$), and $d_{\max} = -d_{\min} = 1$ for the transverse one. This case has been implemented by Margolus on the CAM-6 [9] cellular automata machine, for mildly restricted initial conditions.

With $d_{\min}$ and $d_{\max}$ given for x, y and z, the possible values of each component of the string's momentum range between $-P_{\max}$ and $P_{\max}$, where

$$P_{\max} = (d_{\max} - d_{\min})\frac{N-1}{2}. \tag{2.8}$$

The factor of 2 comes in because only half of the particles move at each time step. The smallest possible variation of momentum for a given string turns out to be

$$\Delta P = 1.$$

Although the momentum can become very large as N increases, the speed of the centre of mass will always be less than or equal to $(d_{\max} - d_{\min})/2$, since the total mass is $N-1$. This is a consequence of the finite range of the rule, which implies a finite speed for the transmission of information through the system.

Similarly, the energy (2.4) has a minimal and a maximal value which are easily calculated by using (2.7). We obtain, for each of x, y and z contributions

$$E_{\min} = \begin{cases} \frac{1}{8}(N-1) & \text{if } a \text{ is half integer} \\ 0 & \text{otherwise} \end{cases}$$

and

$$E_{\max} = \tfrac{1}{8}(N-1)(d_{\max} - d_{\min})^2.$$

It should be noted that, in the particular case where $d_{\min} = 1$ and $d_{\max} = 2$ for the x motion, the energy contribution due to the longitudinal mode is not adjustable but always proportional to the mass ($E_{\min} = E_{\max} = \frac{1}{8}(N-1)$).

Although the above string rule is given in terms of the positions of the particles, it can be translated into a CA rule as soon as $d_{\min}$ and $d_{\max}$ are given. However, it turns out that, under this form, the rule takes a quite complicated expression, and that no natural physical interpretation emerges from that formulation.

2.3. Collisions

So far, we have discussed the propagation of a single free string, i.e. one which does not interact with its surroundings. However, in order to have a true CA model, the rule should be able to deal with an arbitrary initial condition with several strings. This imposes to include in the rule the links that exist between the particles forming each string (a particle must know which string it belongs to). Moreover, when the particles

belonging to different strings want to occupy the same site, or when the trajectories of two or more strings intersect, a collision occurs and we have to modify the evolution rule accordingly. Unfortunately, as we shall see, this program cannot be achieved in the general case with a CA, without violating some constraint.

In addition to collisions between two strings, other situations may be of interest, such as the collision between a string and a point-like particle. This would allow us to model the Brownian motion of a string in suspension in a fluid, or to introduce flexible walls and semipermeable membranes in a lattice-gas fluid.

The idea is to consider interactions that conserve the mass, the momentum and the energy of the entire system. Our purpose is not to give a complete list of all the collisions that can occur, but rather to give the basic relations that describe the exchange of energy and momentum when the motion of the particles in the string is perturbed.

For the sake of simplicity, we shall restrict our attention to perturbations of motion of those particles being updated at time t, say the white ones. Let us denote by $\boldsymbol{q}_i(t+1)$ the position of the ith particle after the collision. Then, we write

$$\boldsymbol{q}_i(t+1) = \boldsymbol{q}_i' + \boldsymbol{\delta}_i \tag{2.9}$$

where $\boldsymbol{q}_i'$ is the position the white particle would have occupied if no collision had occurred. According to (2.1), (2.2) and (2.4), $\boldsymbol{q}_i'$ is

$$\boldsymbol{q}_1' = 2(\boldsymbol{q}_2 - \boldsymbol{a}) - \boldsymbol{q}_1$$

$$\boldsymbol{q}_i' = \boldsymbol{q}_{i-1} - \boldsymbol{q}_i + \boldsymbol{q}_{i+1}$$

or

$$\boldsymbol{q}_N' = 2(\boldsymbol{q}_{N-1} + \boldsymbol{a}) - \boldsymbol{q}_N$$

depending on its position along the string.

Then, using the definition of energy and momentum (equations (2.4) and (2.5)), one can show that the variation of E and $\boldsymbol{P}$ of the string, produced by the $\boldsymbol{\delta}_i$ are

$$\boldsymbol{P}_{\text{final}} - \boldsymbol{P}_{\text{initial}} = \sum_{\text{white}} 2m_i\boldsymbol{\delta}_i \tag{2.10}$$

and

$$E_{\text{final}} - E_{\text{initial}} = \sum_{\text{white}} m_i\boldsymbol{\delta}_i \cdot (\boldsymbol{\delta}_i + \boldsymbol{v}_i') \tag{2.11}$$

where $m_1 = m_N = \frac{1}{2}$, $m_i = 1$ are the masses of the particles and

$$\boldsymbol{v}_i' \equiv \boldsymbol{q}_i' - \boldsymbol{q}_i(t)$$

is the unperturbed velocity.

Clearly, the right-hand sides of (2.10) and (2.11) vanish for $\boldsymbol{\delta}_i = 0$. Moreover, if $\boldsymbol{\delta}_i = -\boldsymbol{v}_i'$, the energy variation is also zero. The reason is because it corresponds to leave the particle at its initial position and this, obviously, does not modify the energy.

As a simple example, let us consider the case of two different interacting strings. More precisely, we shall assume that only the ith particle of the first string collides with the jth one of the second string. The conditions of energy and momentum conservation imply (provided the two particles have the same mass)

$$\boldsymbol{\delta}_i = -\boldsymbol{\delta}_j$$

and

$$\boldsymbol{\delta}_i \cdot (\boldsymbol{\delta}_i + \boldsymbol{v}_i') = -\boldsymbol{\delta}_j \cdot (\boldsymbol{\delta}_j + \boldsymbol{v}_j').$$

One simple solution is

$$2\boldsymbol{\delta}_i = -2\boldsymbol{\delta}_j = \boldsymbol{v}'_j - \boldsymbol{v}'_i. \tag{2.12}$$

If the two particles had opposite velocities before collision (i.e. $\boldsymbol{v}'_j = -\boldsymbol{v}'_i$), one way to satisfy (2.12) is $\boldsymbol{\delta}_i = -\boldsymbol{v}'_i$ and $\boldsymbol{\delta}_j = -\boldsymbol{v}'_j$, which corresponds to keeping the particles in their initial positions. However, in this particular case, no energy is exchanged between the strings. Such an example is illustrated in [6].

Note that another type of collision is also possible, though it is clearly irreversible: when two end particles want to occupy exactly the same position, one lets them do so, and then the two particles form a new particle whose mass is the sum of the individual masses. Since the mass of the end points is precisely half the mass of an internal particle, the result of this kind of collision is to produce one string which is the union of the two previous ones and whose mass, momentum and energy are simply given by the sum of the two initial masses, momenta and energies.

A generalisation of (2.10) and (2.11) can be worked out for the case where both white and black particles undergo collisions during the same time step. In spite of this, it should be noted that, for some configurations, no collisions are possible (for example, when $\boldsymbol{\delta}_i$ is half integer). Therefore, in order to model a system of interacting strings, it is desirable that the particles that are allowed to interact be 'transparent' to each other when collisions cannot occur without violating the conservation laws. This implies that we must relax the exclusion principle (no more than one particle at a given site), which is not very appropriate in a realistic CA implementation. So far, we have not found a tractable way of solving this problem.

On the other hand, the problem of the interaction of a string with point-like particles of a lattice gas is much more simple to deal with because it is easy to make the string transparent to the gas particles when no collisions can take place (string particles and gas particles are of different nature). Moreover, equations (2.10) and (2.11) show that it is indeed possible to define collisions that exchange momentum and energy between a string and the particles of the two-speed HPP model proposed in [10]. It turns out that a transverse string with $d_{\max} = -d_{\min} = 1$ is sufficient to achieve these interactions.

2.4. Some remarks

This string model has two main drawbacks when considering the problem of modelling a non-rigid solid body. First, the strings are one-dimensional objects, which is not the case for a solid. Second, they cannot rotate, or more precisely, the angular momentum is not conserved during the evolution.

The generalisation to objects with more dimensions seems very difficult. So far, our attempts have been unsuccessful. It turns out that some properties of the strings are consequences of the fact that they are one dimensional. For instance, since a particle has only two neighbours, the reflection with respect to their centre of mass also gives a point of the lattice. This fact is no longer true when considering more neighbours.

As far as the problem of conservation of angular momentum is concerned, some improvements can be made. As we shall see in the next section, the reason why angular momentum is not conserved is because $\boldsymbol{a}$ is not zero. Therefore, if we consider the case where $\boldsymbol{a} = 0$, we have the same rule for the three spatial directions, and we obtain a string that can rotate, as shown in figure 4. Of course, in this case one has to relax the condition $d_{\min} = 1$ for the x motion. As a consequence, nothing prevents two

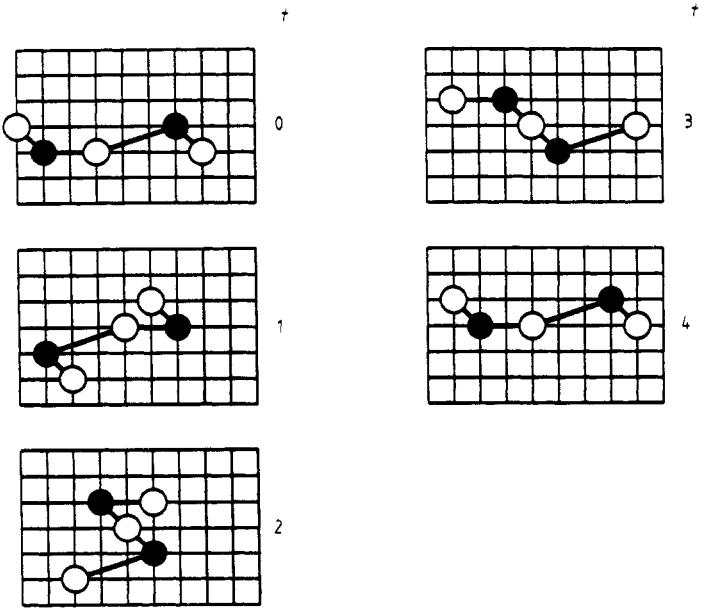

Figure 4. Example of motion where the angular momentum is also conserved ($\boldsymbol{a} = (0; 0)$). The links show the neighbours each particle is connected to. By following the motion, one sees that the two end points of the strings have been interchanged after six time steps. The mass of this string is $M = 6$, its momentum is $\boldsymbol{P} = (0; 0)$, its energy is $E = 11$ and its angular momentum about the centre of mass is $\boldsymbol{L} = (0; 0; 16)$.

particles from occupying the same site and each particle has to keep track of the position of its two nearest neighbours.

Hence, this version of the rule requires a much more complicated scheme of implementation since the exclusion principle does not hold. For this reason, it cannot be extended to a string of arbitrary length. However, the case where $\boldsymbol{a}$ equals zero is interesting because it shows that a system can rotate with a conserved angular momentum, even though the particles are restricted to moving on a square lattice.

3. Discrete-time Hamiltonian equations

The usual way to express a CA rule is to write down an equation for the evolution of the state at each site. However, if the objects we are dealing with are interpreted as composed of particles moving on a lattice, it is sometimes more convenient to return to a description in terms of the positions of these particles, especially when they are distinguishable and their number conserved. As suggested by the previous section, within this framework, our rule has a simple form, and the definitions of physical properties such as centre of mass and total momentum are quite natural. Furthermore, we shall see that the rule can be derived from a discrete-time Hamiltonian formalism, which leads to the expression (2.4) for the total energy. It also gives some hints on how to extend our rule to higher-dimensional objects, while still conserving reasonable physical properties. On the other hand, the drawback of this approach is that it does not guarantee a finite-range rule, in opposition to the traditional description, which is

local by nature. These two ways of describing a system of particles can be compared with the Euler and Lagrange pictures: either we focus our attention on what happens at a given position, or we follow the motion of the particles.

We shall now give the proof of the conservation laws of momentum and energy mentioned in the previous section. For this purpose, we first write the string rule in a more convenient way. Using the fact that the black and white particles alternate along the string and move in succesive steps, the rule given by (2.1) and (2.2), can be cast in the following form, which makes no distinction between the particles, and which is manifestly time reversible:

$$\begin{aligned} &\boldsymbol{q}_1(t-1)-2\boldsymbol{q}_1(t)+\boldsymbol{q}_1(t+1)=2(\boldsymbol{q}_2(t)-\boldsymbol{q}_1(t)-\boldsymbol{a}) \\ &\boldsymbol{q}_i(t-1)-2\boldsymbol{q}_i(t)+\boldsymbol{q}_i(t+1)=\boldsymbol{q}_{i-1}(t)-2\boldsymbol{q}_i(t)+\boldsymbol{q}_{i+1}(t) \\ &\boldsymbol{q}_N(t-1)-2\boldsymbol{q}_N(t)+\boldsymbol{q}_N(t+1)=2(\boldsymbol{q}_{N-1}(t)-\boldsymbol{q}_N(t)+\boldsymbol{a}) \end{aligned} \tag{3.1}$$

where we have labelled the particles along the string from 1 to N, as before. Actually, equations (3.1) are more general than the initial rule. In order to be equivalent to (2.1) and (2.2), they should be completed with the appropriate initial conditions at times t and $t+1$ expressing that, in fact, only the white or the black particles can move at a given time. However, the results we are going to derive are also valid without this restriction.

In addition, it should be noted that the term $\boldsymbol{q}_i(t)$ is not necessary in these equations, since it shows up with the same factor on both the right-hand side and the left-hand side. We have kept it in order to make the left-hand side look like the discrete second-order time derivative operator. It turns out that the fact that the rule does not depend on $\boldsymbol{q}_i(t)$ itself makes possible the alternating motion of the black and white particles. As we shall see, the consequence of this is that the particles will never be too far from each other. Unfortunately, this property is not satisfied when considering a natural extension of (3.1) to higher-dimensional objects.

Let us now introduce the following Hamiltonian:

$$H(\boldsymbol{p}_1,\ldots,\boldsymbol{p}_N,\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N)=\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{2m_i}+U(\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N) \tag{3.2}$$

where $\boldsymbol{p}_i$, $\boldsymbol{q}_i$ and m_i are, respectively, the momentum, the position and the mass of the ith particle of the string.

We now define the discrete-time equations of motion as

$$\boldsymbol{q}_i(t+1)-\boldsymbol{q}_i(t)=\frac{\partial H}{\partial \boldsymbol{p}_i}=\frac{1}{m_i}\boldsymbol{p}_i(t) \tag{3.3}$$

and

$$\boldsymbol{p}_i(t)-\boldsymbol{p}_i(t-1)=-\frac{\partial H}{\partial \boldsymbol{q}_i}=-\frac{\partial U(t)}{\partial \boldsymbol{q}_i}. \tag{3.4}$$

The only modification to the usual Hamiltonian equations is that the time derivative is replaced by a finite difference. Note, however, the important fact that the time arguments are not the same for position and for momentum. This ensures the time reversibility of the evolution, as can be seen by substituting (3.3) into (3.4). Indeed,

we obtain the following equation of motion:

$$\boldsymbol{q}_i(t+1)-2\boldsymbol{q}_i(t)+\boldsymbol{q}_i(t-1)=-\frac{1}{m_i}\frac{\partial H(t)}{\partial \boldsymbol{q}_i}. \tag{3.5}$$

Now, if we choose

$$m_1=\tfrac{1}{2}m_2=\ldots=\tfrac{1}{2}m_{N-1}=m_N=\tfrac{1}{2} \tag{3.6}$$

and

$$U(\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N)=\frac{1}{2}\sum_{i=1}^{N-1}(\boldsymbol{q}_{i+1}-\boldsymbol{q}_i-\boldsymbol{a}_i)^2 \tag{3.7}$$

equation (3.5) reduces exactly to our rule (3.1). It should be noted that, in the above relations, the space derivatives are the usual ones. In fact, equation (3.1) does not refer to a discrete space. It is just a matter of properly choosing the initial configuration of the string to ensure that it will stay on a lattice. As a consequence, the proof of the conservation of momentum has the same flavour as in the usual continuous time Hamiltonian formalism: we define

$$\boldsymbol{P}(t)=\sum_{i=1}^{N}\boldsymbol{p}_i(t). \tag{3.8}$$

From equation (3.4), we have

$$\boldsymbol{P}(t)-\boldsymbol{P}(t-1)=-\sum_{i=1}^{N}\frac{\partial U}{\partial \boldsymbol{q}_i}.$$

The left-hand side of this equation reduces to zero if U is invariant under any continuous space translation $\boldsymbol{r}$, as can be seen by differentiating

$$U(\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N)=U(\boldsymbol{q}_1+\boldsymbol{r},\ldots,\boldsymbol{q}_N+\boldsymbol{r})$$

with respect to $\boldsymbol{r}$.

Since our potential (3.7) clearly satisfies this property, momentum will be a constant during the evolution of the string. In addition, by summing (3.3) over i, we obtain the expected relation for the speed of the centre of mass, namely

$$\frac{1}{M}\sum_{i=1}^{N}m_i\boldsymbol{q}_i(t+1)-\frac{1}{M}\sum_{i=1}^{N}m_i\boldsymbol{q}_i(t)=\frac{1}{M}\boldsymbol{P}.$$

In a similar way, we could prove that the angular momentum $\boldsymbol{L}=\Sigma\,\boldsymbol{q}_i\times\boldsymbol{p}_i$ is conserved if H is invariant under rotations. Therefore, as already mentioned in the previous section, our strings can rotate when U is invariant under rotations, i.e. when $\boldsymbol{a}=0$.

The problem of energy conservation is not so obvious. Indeed, time is intrinsically discrete and we do not expect the usual proof to work. However, it turns out that for a harmonic potential it is still possible to associate a conserved quantity with our Hamiltonian, that we are going to interpret as the energy of the system.

Let us first define the 'kinetic energy' T as

$$T(t)=\sum_{i=1}^{N}\frac{\boldsymbol{p}_i(t)\cdot\boldsymbol{p}_i(t-1)}{2m_i}. \tag{3.9}$$

We can now calculate the kinetic energy change after one time step. According to its definition and equation (3.3), we have

$$
\begin{aligned}
&T(t)-T(t-1)\\
&\quad=\sum_{i=1}^{N}\frac{m_i}{2}[(\boldsymbol{q}_i(t+1)-\boldsymbol{q}_i(t))\cdot(\boldsymbol{q}_i(t)-\boldsymbol{q}_i(t-1))\\
&\qquad-(\boldsymbol{q}_i(t)-\boldsymbol{q}_i(t-1))\cdot(\boldsymbol{q}_i(t-1)-\boldsymbol{q}_i(t-2))]\\
&\quad=\tfrac{1}{2}\sum_{i=1}^{N}m_i(\boldsymbol{q}_i(t)-\boldsymbol{q}_i(t-1))\cdot[\boldsymbol{q}_i(t+1)-2\boldsymbol{q}_i(t)+\boldsymbol{q}_i(t-1)\\
&\qquad+\boldsymbol{q}_i(t)-2\boldsymbol{q}_i(t-1)+\boldsymbol{q}_i(t-2)]\\
&\quad=\tfrac{1}{2}\sum_{i=1}^{N}(\boldsymbol{q}_i(t)-\boldsymbol{q}_i(t-1))\cdot\left(-\frac{\partial U(t)}{\partial \boldsymbol{q}_i}-\frac{\partial U(t-1)}{\partial \boldsymbol{q}_i}\right).
\end{aligned}
\tag{3.10}
$$

In order to find out the conditions the potential should satisfy to have a conserved energy, we assume that U is given by a polynomial expression of the $\boldsymbol{q}_i$. It is then convenient to write U as

$$U=U_0+U_1+\ldots+U_l+\ldots \tag{3.11}$$

where U_0 is a constant, U_1 a linear function of the coordinates and, more generally, U_l is a homogeneous function of order l:

$$U_l(\mu\boldsymbol{q}_1,\ldots,\mu\boldsymbol{q}_N)=\mu^l U_l(\boldsymbol{q}_1,\ldots,\boldsymbol{q}_N).$$

Using Euler's relation, the U_l obey

$$lU_l=\sum_{i=1}^{N}\boldsymbol{q}_i\cdot\frac{\partial U_l}{\partial \boldsymbol{q}_i}. \tag{3.12}$$

Now, with (3.11) and (3.12), we can rewrite (3.10) as

$$
\begin{aligned}
&T(t)-T(t-1)\\
&\quad=-\frac{1}{2}\sum_l lU_l(t)+\tfrac{1}{2}\sum_l lU_l(t-1)\\
&\qquad+\frac{1}{2}\sum_{i=1}^{N}\sum_l\left(\boldsymbol{q}_i(t-1)\cdot\frac{\partial U_l(t)}{\partial \boldsymbol{q}_i}-\boldsymbol{q}_i(t)\cdot\frac{\partial U_l(t-1)}{\partial \boldsymbol{q}_i}\right).
\end{aligned}
\tag{3.13}
$$

In order to obtain a quantity that is conserved during the evolution, the right-hand side of this equation should be an expression taken at time t minus the same expression taken at time $t-1$. Therefore, the double sum should vanish, at least for the $\boldsymbol{q}_i$ belonging to the lattice.

To check that our potential (3.7) indeed verifies this property it is convenient to write (3.13) in a different form. First, since U_1 is a linear function, its first derivative is a constant that does not depend on t. Consequently, we have

$$\boldsymbol{q}_i(t)\cdot\frac{\partial U_1(t-1)}{\partial \boldsymbol{q}_i}=\boldsymbol{q}_i(t)\cdot\frac{\partial U_1(t)}{\partial \boldsymbol{q}_i}$$

and

$$\boldsymbol{q}_i(t-1)\cdot\frac{\partial U_1(t)}{\partial \boldsymbol{q}_i}=\boldsymbol{q}_i(t-1)\cdot\frac{\partial U_1(t-1)}{\partial \boldsymbol{q}_i}.$$

Second, U_2 is a quadratic function and its first derivative is linear. Then, by symmetry, it is easy to show that

$$\sum_{i=1}^{N}\left(\boldsymbol{q}_i(t-1)\cdot\frac{\partial U_2(t)}{\partial \boldsymbol{q}_i}-\boldsymbol{q}_i(t)\cdot\frac{\partial U_2(t-1)}{\partial \boldsymbol{q}_i}\right)=0.$$

Finally, after some algebra, (3.13) is

$$\begin{aligned}T(t)+U_0+U_1(t)+U_2(t)+\sum_{l>2} lU_l(t)&\\ =T(t-1)+U_0+U_1(t-1)+U_2(t-1)+\sum_{l>2} lU_l(t-1)&\\ +\frac{1}{2}\sum_{i=1}^{N}\sum_{l>2}\left(\boldsymbol{q}_i(t-1)\cdot\frac{\partial U_l(t)}{\partial \boldsymbol{q}_i}-\boldsymbol{q}_i(t)\cdot\frac{\partial U_l(t-1)}{\partial \boldsymbol{q}_i}\right).&\end{aligned}$$

Thus, when U_l is zero for every $l>2$, the total energy E can be defined as the sum of the potential and kinetic energies:

$$E(t)=T(t)+U(t). \tag{3.14}$$

This is precisely the case for U given by (3.7). Therefore our string model satisfies the energy conservation law

$$E(t)=E(t-1). \tag{3.15}$$

Relation (3.15) is then valid only for a harmonic potential U, given by the sum of a linear and a quadratic expression in the coordinates. The remarkable fact is that (3.14) is very similar to the Hamiltonian that generated the equations of motion (3.3). The only difference between $E(t)$ and $H(t)$ is the form of the kinetic energy, which contains the product $\boldsymbol{p}_i(t)\cdot\boldsymbol{p}_i(t-1)$, instead of the usual $\boldsymbol{p}_i^2(t)$ term. As a consequence, the kinetic energy can be negative, which is not very satisfactory from a physical point of view. However, in the particular implementation discussed in section 2, since the particles only move once every two steps, the kinetic energy T always vanishes and (3.14) reduces to (2.4):

$$E(t)=U(t).$$

The fact that $T=0$ has the interesting consequence that the particles forming the string cannot spread out indefinitely, because U is a constant.

It is interesting to note that E can be rewritten in a different way when the potential takes the form (3.7). For the sake of simplicity, we illustrate the point for one spatial dimension. By expanding the sum and rearranging the terms, we have

$$\begin{aligned}\sum_{i=1}^{N-1}(x_{i+1}-x_i-a)^2&\\ =\sum_{i=1}^{N-1}(x_{i+1}^2-2x_{i+1}x_i+x_i^2)-2a\sum_{i=1}^{N-1}(x_{i+1}-x_i)+(N-1)a^2&\\ =\sum_{i=2}^{N-1}(x_i^2-x_{i+1}x_i-x_ix_{i-1}+x_i^2)+x_1^2+x_N^2-x_1x_2-x_{N-1}x_N&\\ -2a(x_N-x_1)+(N-1)a^2&\\ =x_1(x_1-x_2+a)+\sum_{i=2}^{N-1}[x_i(2x_i-x_{i-1}-x_{i+1})]+x_N(x_N-x_{N-1}-a)&\\ +a(x_1-x_N)+(N-1)a^2.&\end{aligned}$$

Hence, using the equations of motion (3.1), we obtain

$$\sum_{i=1}^{N-1}(x_{i+1}(t)-x_i(t)-a)^2$$

$$=-\sum_{i=1}^{N} m_i x_i(t)(x_i(t-1)-2x_i(t)+x_i(t+1))$$

$$+a(x_1(t)-x_N(t))+(N-1)a^2$$

and finally

$$T(t)+U(t)=\frac{1}{2}\sum_{i=1}^{N} m_i(x_i^2(t)-x_i(t-1)x_i(t+1))$$

$$+\tfrac{1}{2}a(x_1(t)-x_N(t))+\tfrac{1}{2}(N-1)a^2. \tag{3.16}$$

It turns out that, for $a=0$, this expression is similar to the energy proposed by Chen *et al* [11] in their CA model for waves.

The results of this section raise the question of how to generalise equation (3.14) to a non-harmonic potential. One might ask whether or not a Hamiltonian-like formalism could be developed that would describe other discrete mechanical systems (a lattice-gas dynamics, for example). Although our derivation does not constitute a general proof, it is an indication that the answer may be negative.

Apparently, the problem of finding the additive dynamical invariants in a discrete system is difficult since Noether's theorem does not apply, and each rule must be investigated separately. Note that, in our case, the dynamics of the system can be reduced to a problem of propagation and reflection of waves (see next section). Therefore, the invariants can be obtained from the explicit solution. In particular, an invariant similar to the one Pomeau discovered [12] for the Q2R rule of Vichniac can be defined in our model, but it does not correspond to an interesting physical property.

4. Propagation of sound waves

It turns out that the motion of the string arises due to the transmission and reflection of one longitudinal and two transverse sound waves. These waves propagate along the string and are totally reflected at the end points. This fact will be illustrated for the longitudinal x motion (the same derivation applies to the transverse modes). Let us introduce

$$\Delta_i = x_{i+1}-x_i-a \tag{4.1}$$

which describes the elongation of the 'springs' linking particles i and $i+1$. When all Δ_i are zero, the state of the string does not change. Note that Δ_i cannot be zero for an implementation where a is half integer.

In terms of Δ_i, the equations of motion (3.1) are

$$\Delta_1(t+1)-2\Delta_1(t)+\Delta_1(t-1)=\Delta_2(t)-3\Delta_1(t) \tag{4.2}$$

$$\Delta_i(t+1)-2\Delta_i(t)+\Delta_i(t-1)=\Delta_{i-1}(t)-2\Delta_i(t)+\Delta_{i+1}(t) \tag{4.3}$$

$$\Delta_{N-1}(t+1)-2\Delta_{N-1}(t)+\Delta_{N-1}(t-1)=\Delta_{N-2}(t)-3\Delta_{N-1}(t). \tag{4.4}$$

This set of equations corresponds to a new CA rule for the propagation of sound in the string. Although they look like the equations describing the positions of the particles

in the string, they have the advantage of being local for any initial configurations. Indeed, if we are not interested in the motion of the particles but in the spacings between them, the index i can just as well refer to a definite site of the CA and Δ_i to its state.

The second interesting property of this rule is that equation (4.3) admits a very simple set of solutions, namely

$$\Delta_i(t) = f(i-t) + g(i+t). \tag{4.5}$$

This can be seen by direct substitution of (4.5) into (4.3). Therefore, (4.3) is not only a discrete version of the wave equation, it actually describes waves moving forward and backward with unit speed.

However, if the string is neither infinite nor periodic, we also have to take into account (4.2) and (4.4). It is easy to see what happens at the end points by considering a pulse travelling for instance to the left, defined by $\Delta_i(t-1) = \Delta_i(t) = 0$ for all i, except for $i = i_0$ for which $\Delta_{i_0+1}(t-1) = \Delta_{i_0}(t) = \Delta$. Successive applications of the above rule show that the pulse is reflected with the opposite sign when it reaches the left end of the system. This fact suggests writing equations (4.2), (4.3) and (4.4) in a more unified way, by using reflection and transmission coefficients. By demanding that the two moving waves $f(i, t)$ and $g(i, t)$ obey

$$f(i, t+1) = T_{i-1}^{i} f(i-1, t) + R_i^{i-1} g(i, t) \tag{4.6}$$

and

$$g(i, t+1) = T_{i+1}^{i} g(i+1, t) + R_i^{i+1} f(i, t) \tag{4.7}$$

we obtain for $\Delta_i(t) = f(i, t) + g(i, t)$

$$\begin{aligned}\Delta_i(t+1) - 2\Delta_i(t) + \Delta_i(t-1) \\ = T_{i-1}^{i}\Delta_{i-1} + (R_i^{i+1} + R_i^{i-1} - 2)\Delta_i + T_{i+1}^{i}\Delta_{i+1}\end{aligned} \tag{4.8}$$

where $T_i^{i\pm1}$ and $R_i^{i\pm1}$ respectively denote the transmission and reflection coefficients of a wave propagating from site i to site $i \pm 1$. In order to derive (4.8), equations (4.6) and (4.7) have to be completed with the usual relations (see [13], for instance)

$$T = 1 + R \qquad \text{and} \qquad R_i^{i\pm1} = -R_{i\pm1}^{i}.$$

The values of R and T that correspond to the string motion are $R = 0$, $T = 1$ for the internal points, and $R = -1$ and $T = 0$ for the end points. Another interesting case (in fact, the complementary case) is $R = 1$ and $T = 2$, which describes a fixed end point and a transmitted wave in the medium this end point is attached to. In this case, there is no overall motion of the string, but rather an oscillation of its centre of mass.

Intermediate cases $-1 < R < 0$ and $0 < R < 1$ would be interesting too, but they generate non-integer numbers, which is not desirable for a CA.

Finally, we would like to emphasise that the implementation of the string rule in terms of black and white particles moving alternately corresponds to specific $f(i-t)$ and $g(i+t)$, having the following properties:

$$f(k) = \begin{cases} f(k) & \text{if } k \text{ is even} \\ 0 & \text{if } k \text{ is odd} \end{cases} \tag{4.9}$$

$$g(k) = \begin{cases} 0 & \text{if } k \text{ is even} \\ g(k) & \text{if } k \text{ is odd.} \end{cases} \tag{4.10}$$

The wave propagation is then simply achieved by pairing adjacent sites two by two, interchanging their contents and then performing the same operation on the alternate partition.

5. Conclusions

In this paper, we have proposed a discrete mechanical model of one-dimensional objects that move with adjustable mass, momentum and energy in a three-dimensional space. This model is efficiently described by a cellular automata rule when considering some restricted situations, namely (i) a single free string that cannot rotate, (ii) a system of purely longitudinal interacting strings with $d_{\min} = 1$, $d_{\max} = 2$, and such that the near ends of adjacent strings are all terminated by the same colour of particle: in this case, the interactions can only occur between the end points and the type of collisions described in section 2 are always possible since the end points have equal or opposite velocities. And finally, (iii) the case of a string interacting with point-like particles, like the ones of a lattice-gas model.

Unfortunately, due to the exclusion principle inherent in a cellular automata, a realistic implementation of both the rotating string and a general system of interacting strings cannot be carried out without breaking the conservation laws of mass, momentum or energy. And even more serious difficulties arise when considering generalisations to two- or three-dimensional objects. Therefore, a completely satisfactory CA model of non-rigid moving solid bodies is still to be devised. Our approach, which is a first attempt in this direction, illustrate some of the typical difficulties encountered in order to achieve such a program. Although these difficulties are due to some fundamental limitations proper to cellular automata, some improvements could be made by considering a different physical interpretation, more closely related to the nature of the cellular automata description.

Nevertheless, in its present form, our model has several possible applications to physical problems. For instance, the possibility of having interactions between point-like particles and a string allows us to consider the case of a linear molecular chain in suspension in a fluid. One may expect that the motion of the centre of mass of such a chain will be described by a mobility μ and will obey a Langevin equation whose parameters are determined by the interactions with the surrounding fluid. The complete analysis of the motion of the string is an interesting problem that will be investigated soon with numerical simulations.

In relation to this problem, it should be noted that a string can be used as a thermometer for a multi-speed lattice gas model of a fluid: assuming a canonical distribution of the energy, the behaviour of the string in equilibrium with the lattice-gas particles provides a new way to define the temperature of the fluid. This method of measuring the temperature has the advantage of being in the spirit of the CA approach, because the thermometer is itself a part of the system, as is the case in a real experiment. Also, this new prescription of defining the temperature in a lattice-gas fluid may have some interesting theoretical implications when it is compared with the two more direct, but unequal, temperature scales given by the equipartition of energy and by the microcanonical ensemble. Moreover, this method can be used to measure a local temperature in non-equilibrium situations, provided the length of the string is appropriate.

Furthermore, our strings provide a simple microscopic model of a one-dimensional solid body which can be relevant in non-equilibrium statistical mechanics. Efficient numerical simulations can be performed in order to study the probability distribution in a non-equilibrium situation, when the two extremities of a string are brought into contact with two reservoirs having different temperatures. Heat flow and thermal conductivity could be measured.

In addition to the above problems which will be discussed in detail in a forthcoming paper, it would be interesting to use a string interacting with a lattice-gas fluid as a model of a linear polymer in a solvent. Indeed, our string model is not very different from the models proposed to describe the dynamics of an ideal polymer [14]. However, it requires us to consider only some restricted situations because our dynamics does not allow for loops along the string.

Moreover, it is certainly desirable to deal with several polymers in order to simulate real physical situations. Although our model is not yet appropriate for considering a system of several interacting strings, some improvements can be realised, as suggested by Bar-Yam [15, 16]. Indeed, if one focuses attention solely on the polymers and not on the polymer–solvent system, the only conservation law which really matters is the conservation of the number of particles, since the strings can exchange momentum and energy with the solvent. In this case, the only constraint we are left with is to define a set of rules that preserve the integrity of each chain.

Acknowledgments

I would like to thank Tommaso Toffoli and Norman Margolus for having inspired this research, and Mark A Smith for stimulating discussion and careful reading of the manuscript. This work was supported by the Swiss National Science Foundation.

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