A "wave automaton" for wave propagation in the time domain: I. Periodic systems

Patrick Sebbah, Didier Sornette, Christian Vanneste

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A « wave automaton » for wave propagation in the time domain : I. Periodic systems

Patrick Sebbah, Didier Sornette and Christian Vanneste

Laboratoire de Physique de la Matière Condensée (*), Université de Nice-Sophia Antipolis, Parc Valrose, B.P. 71, 06108 Nice Cedex 2, France

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Abstract. — In Vanneste *et al.*, *Europhys. Lett.* **17** (1992) 715, a new lattice model was introduced for the *dynamical* propagation of waves in arbitrary heterogeneous media, which is efficient for calculations on large systems (1 024 × 1 024) over long times (several 10^6 inverse band widths). Instead of starting from a wave equation or a Hamiltonian which needs to be discretized for numerical implementation, the model is defined by the set of S-matrices, one for each node, describing the interaction of the wave field with the scatterers. Here, we expose in detail the general method of construction of the S-matrices and discuss the physical meaning of the dynamical S-matrix approach. We calculate the properties of this model for a class of parameters in the periodic case and exhibit the form of the Bloch modes, the dispersion relation and the mode density. In a companion paper, we study the transport of wave packets in arbitrary random media.

1. Introduction.

The propagation of waves in arbitrary linear systems can be characterized essentially by three quantities : the spectrum, the spatial proper modes and the time dependent response. Description of waves in the Fourier domain is by far the most developed in comparison with the time domain. The Fourier domain is physically meaningful and particularly efficient for the treatment of homogeneous or weakly heterogeneous systems. The present understanding of the behavior of waves in strongly disordered media, notably in the presence of wave localization [1-3], relies essentially on a description in the Fourier domain. In this way, the hallmarks of wave localization is the appearance of spatially localized proper modes and a pure point spectrum. More generally, Anderson localization is usually described in terms of specific properties of the stationary wave at a given frequency. On the other hand, much less attention [4] has been devoted to the dynamical properties of wave localization, for example the manner in which waves become localized as a function of time from an initial propagating

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state. Since both the wave and Schrödinger equations are linear, wave dynamics can be formally deduced from the knowledge of the frequency dependence of the stationary problem (see for instance [5, 6] for the wave localization problem). However, the interest in investigating wave dynamics directly (in particular in the strong disorder regime) is that it can exhibit more clearly some striking features of the phenomenon in that it provides a genuine real space-time representation. Furthermore, localization dynamics determine many important properties of the energy wave transport in random systems, such as transient injection transmissions or currents, hopping kinetics, pulse transmission and reflections [7a], . Along these directions, recent experimental studies on acoustic waves [7b] using fast electronics and large transducer arrays have demonstrated the possibility of returning in time ($t \to T - t$) a narrow wave packet, thus enabling for instance the spontaneous focalization on a specific target of a pulse propagating through arbitrary heterogeneous media. Another particularly significant domain where wave propagation in the time domain is important is seismology : the challenge here is to analyse finite wave signals and deduce from then the heterogeneous structure of the earth and/or the source mechanism (nature of the rupture) of the seismic waves created during earthquakes. In engineering these problems are encountered for instance in the non-destructive Emission Acoustic technique [8]. More generally, the possibility of having access to the time domain suggests a wealth of techniques to treat, filter, etc., the wave and thus gain useful information on the source or the carrying medium.

Analysis of wave propagation in the time domain has been studied previously essentially by using various numerical schemes, starting from the Schrödinger parabolic equation $i\,\partial\Psi/\partial t = H\Psi$ (we note « i » the square root of -1), the hyperbolic wave equation $c^{-2}\,\partial^2\Psi/\partial t^2 = \Delta\Psi/n(\mathbf{r})$, etc. In these equations, H is the Hamiltonian and $n(\mathbf{r})$ is the local index of refraction. A first difficulty of numerical schemes comes from the discretization of space and time, which leads to spurious dispersion relations at high frequency and wavevectors. A more serious problem is that the numerical schemes must preserve the norm of the wave function, i.e. the time evolution operator $U(t) = \exp[-itH]$ (for the Schrödinger equation) must be unitary. Approximate methods of integration, such as the standard implicit Crank-Nicholson method [9, 10] have been introduced to approximate the time evolution operator. Recently, more accurate and efficient algorithms have been proposed [11-13].

The approach discussed in the present paper (see also [14] for a preliminary account), although related to explicit integration schemes of the wave equations, starts from an entirely different point of view. This approach has initially been introduced a few years ago for the computation of *stationary* transmissions in random media [15], where its potential for calculating *time-dependent* wave properties has been overlooked. We have recently rediscovered it from a different approach [14] and extended it for studying time-dependent wave propagation in large heterogeneous media at long times. Its main qualities are to be inherently explicit, highly parallel and inconditionally stable while conserving the energy flux exactly. It is probably the simplest direct approach one can think of to deal with the general problem of the time evolution of a wave in an arbitrary medium. Its simplicity stems from the fact that it treats directly the impinging waves on each node of a lattice and describes the scattering event, in the time domain, by a scattering matrix (S-matrix) one for each node. In contrast to standard approaches using S-matrices, it is important to stress that we use it in the time domain. We do not really attempt *a priori* to model a specific wave equation, but our goal is to define the minimal ingredients that must be kept in order to model a wave. They are 1) to deal with complex fields $A\,e^{i\phi}$, 2) to obey the condition of energy conservation or equivalently of wave function norm conservation and 3) to satisfay the invariance with respect to time-reversal (in the absence of a magnetic field for electrons or more generally of a rotational field coupled to the wave field). In a sense, our purpose for « computing » is insight, not numbers [16]. Then, due to its modelling philosophy, the « wave automaton » appears to be an ideal starting point

for the development of numerical routines for the computation of more general propagation processes.

The « wave automaton » is in some respect similar in spirit to the cellular automata models [17], in that macroscopic equations are modelled by arrays of variables that follow local interaction rules. Similarly to our guideline in the construction of the « wave automaton », cellular automata have been proposed as alternative to, rather than an approximation of, partial differential equations in modelling physics. In the standard cellular automata models introduced to model fluid dynamics [18], the dynamical variables are typically limited to just a few states (for instance, Boolean variables), hence the name « automaton » in the sense of Von Neumann, and the macroscopic partial differential equation is recovered after a suitable time and space averaging is taken. Since acoustic waves derive from the complete compressible Navier-Stokes equation, a similar approach can be proposed for modeling waves [19]. However, one needs again to average over many lattice sites and time steps to get rid of fluctuations and to recover the macroscopic wave equation, which limits the useful size and the time span of the dynamics. On the contrary, our « wave automaton » uses continuous complex variables $A\,e^{i\phi}$, which allows us to avoid the averaging procedure since the wave field components must be considered as discrete realizations of their macroscopic counterparts. Note that we use the term « automaton » in the broader pre- Von Neumann sense of an artificial « creature » (here the complex field) imitating real life (the wave), and not in the restricted meaning of a Boolean or discrete variable.

Enders has recently commented [20] that 1) there is a physical (Huygens') principle underlying the « wave automaton » approach presented in reference [14] and in this paper and 2) there is a physical (network) representation/realization model for such numerical algorithms/routines. In the term Huygens' principle, are comprised 1) the principle of action-by-proximity and 2) the superposition of secondary wavelets according to the smoothness properties of the field under consideration.

In section 2, we expose in detail the general method of construction of the S-matrices, and discuss the physical meaning of the S-matrix approach. In section 3, we calculate the properties of this model for a class of parameters defining the wave automaton in the periodic case and exhibit the form of the Bloch modes, the dispersion relation and the mode density. Appendix A gives the relation between the scattering matrix (S-Matrix) representation and the usual transfer matrix (T-Matrix) representation. Appendix B provides a list of the different possible sets of parameters for the parametrisation of S-Matrix that describes isotropic scattering. In the following paper [21], we use the « wave automaton » to study the properties of the dynamical transition of a wave packet into a localized state.

2. Description of the « Wave Automaton »

3.1 GENERAL CASE. — Consider a d-dimensional discrete lattice of size L^d and unit mesh size. We will consider square ($d = 2$), cubic ($d = 3$) or more generally hypercubic lattices, such that the number of bonds connecting to a given node is $z = 2\,d$. Consideration of other lattice symmetries is straightforward using the corresponding S-matrices for the corresponding coordination number z (see below). Two scalar waves (each described by a modulus and phase) can propagate in opposite directions along each bond of this lattice. Since time dependent processes are studied, the waves are in fact pulses which interact with the nodes (the scatterers) at discrete times. It may be useful to look at this system as a simplified representation of a physical network of unidimensional waveguides connected at each node of the lattice, such that the wave locally travels unidimensionally in each guide and is coupled to transverse directions at the connecting nodes. Again, in contrast to previous works [22-24] on waveguides, only pulses, and not stationary waves, propagate in our model.

It is important to note that for the square lattice in 2D, or for the cubic lattice in 3D and more generally for hypercubic lattices in arbitrary dimensions, the network can be divided into two separate alternate cubic lattices (see Fig. 1 for the 2D case). At each scattering event by the nodes of the network, one can distinguish the waves ($\rightarrow \leftarrow$) which are impinging upon the nodes and those ($\leftarrow \rightarrow$) which are going away from the nodes. Then, the propagation is the superposition of two independent propagations, one for the impinging waves and the other for the outgoing waves. One can easily be convinced that the propagation of one of these waves, when described every two time steps, remains always either on the white or on the black sublattice (see Fig. 1). The other sublattice is only present to connect the nodes of the first sublattice at the intermediate odd time steps. These properties do not hold for other topologies such as the triangular lattice in 2D. In the following, we will restrict our attention to cubic lattices. Therefore, in practice, we can either use the full dynamics calculated every time step or half of it every two time steps. The results that will be presented on the dispersion relation and density of states concerns the dynamics observed on one of the sublattices every two time steps.

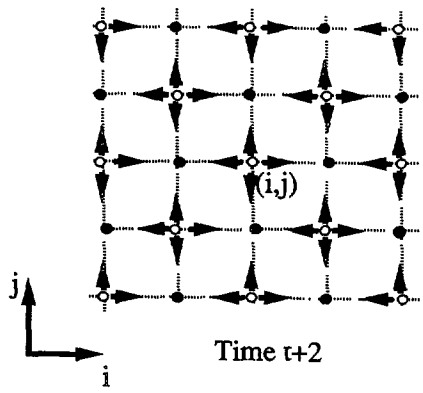

Fig. 1. — Representation of the two independent sublattices present in the square lattice geometry. Four waves are escaping from node (i, j) at time t. At time $t + 2$, these waves and their counterparts are found only on the white nodes.

At a given time t^-, 2d waves along the 2d bonds connected to a given node are impinging on this node (scatterer). 2d waves emerge at time t^+ from this node after the scattering process (see Fig. 2). The scatterer located on each node of the lattice thus allows the coupling of all the different directions of propagation. Mathematically, the scatterer is represented by a 2d by 2d scattering-matrix (4 by 4 for a two-dimensional lattice) which transforms the 2d fields reaching a node into the 2d outcoming fields. The $d = 2$ case is depicted in figure 2a which gives the convention for the four components of both the impinging and outgoing fields. This operation is supposed to be instantaneous (between t^- and t^+). Each outcoming pulse at time t^+ then propagates at constant unit speed along its bond towards the neighboring node to become at time $t + 1$ an incoming field on this node. Our notation is : bond 1 of node (i, j) is bond 2 of node $(i, j - 1)$; bond 3 of node (i, j) is bond 4 of node $(i - 1, j)$; bond 2 of node (i, j) is bond 1 of node $(i, j + 1)$; bond 4 of node (i, j) is bond 3 of node $(i + 1, j)$; see Fig. 2a).

Up to now, the definition of the model does not specify a wave propagation. In fact, all the physics is contained in the scattering-matrix which transforms the 2d fields reaching a node

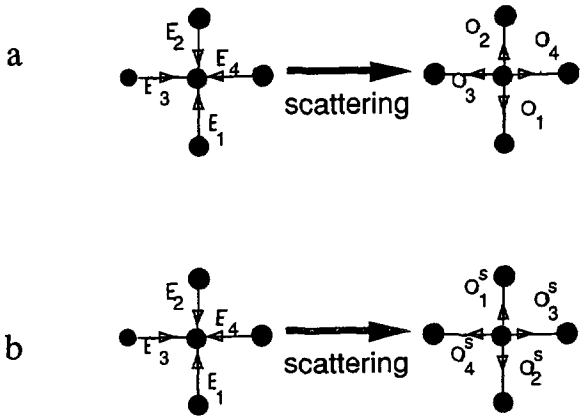

Fig. 2. — Scattering process at a node of the square lattice. a) Scattering process at a node of the square lattice and definition of our parametrization. b) Parametrization of the scattering process leading to the standard S-matrix.

into the 2d outcoming fields. Of course, nor any 2d by 2d matrix is allowed. In order to represent a wave, one must constraint the S-matrices in order that the two fundamental properties of the propagation of a wave are obeyed : 1) the conservation of energy flux and 2) the time reversal invariance. These two conditions ensure the fundamental characteristic of waves to interfere. Such constraints can also be considered as symmetries that the S-matrix must obey and are known to control its structure [25].

For d-dimensional systems, we can note E (resp. O) the column vector of the incident (resp. outgoing) fields. We can thus write more generally

$$O = S \,.\, E \,. \tag{1}$$

The condition of conservation of the energy flux reads ${}^{t}O^{*}\ O = {}^{t}E^{*} \,.\, E$ (${}^{t}E$ means transposed of E and E^{*} the complex conjugate of E), with ${}^{t}O^{*} \,.\, O = {}^{t}E^{*}\ {}^{t}S^{*}\ S \,.\, E$, using (1). The equality being true for any field E, this leads to the condition ${}^{t}S^{*}\ S = \mathbb{1}$ (where $\mathbb{1}$ is the unit matrix), thus expressing the fact that the S-matrix is unitary [25, 26].

Under time reversal, O is changed into E^{*} which is now the incident field, and E into O^{*} which now the outgoing field. Invariance with respect to time reversal thus reads

$$E^{*} = S \,.\, O^{*} \tag{2}$$

i.e. the same S-matrix transforms the time reversed fields. Equation (2) also reads $O = S^{*-1} \,.\, E = {}^{t}S \,.\, E$ since $S^{*-1} = {}^{t}S$ by the unitarity. For this equation to be compatible with the definition (1) of the S-matrix, this leads to ${}^{t}S = S$, i.e. the S-matrix defined above is symmetric.

Note that our convention, for the channels of the outgoing field O, differs from the standard definition leading to the standard parametrization of the S-matrix. In figure 2a, we associate an index to each bond linking a node to its neighboring nodes. This index thus controls the index of the components of both the incident and the outgoing fields. In contrast, in the standard definition of a S-matrix, the index of the outgoing field component is defined by the direction of the incident field (see Fig. 2b). In other words, the standard definition of the scattered field O^{s} is deduced from our parametrization O by a coordinate inversion. If we note P the operator for the coordinate inversion, we then have $O^{s} = P \,.\, O = P \,.\, S \,.\, E \equiv S^{s}\ E$, thus

defining the standard S-matrix $S^s = P \,.\, S$. From ${}^tS = S$ with $S = P \,.\, S^s$, since $P^{-1} = P$, this leads to ${}^tS^s \,.\, {}^tP = P \quad S^s$, i.e.

$$P \,.\, {}^tS^s \,.\, P = S^s \,, \tag{3}$$

since ${}^tP = P$. Expression (3) is the standard condition for an S-matrix as defined in textbooks [26]. In the sequel, we will use the notation of figure 2a such that our S-matrix is unitary and *symmetric*.

Note that in order to treat the case of electrons in scattering media in the presence of a magnetic field, we need to relax the condition of time reversal invariance in favor of the weaker constraint that the phases of time reversed scattering events possess opposite signs. This interesting problem is not investigated in the present work.

The two conditions of unitarity and symmetry that S-matrix must obey imply that it is parametrized by exactly $d(2\,d + 1)$ free real parameters [27] (instead of $8\,d^2$ real parameters for arbitrary $2\,d \times 2\,d$ matrices with complex coefficients). This gives 10 (resp. 21) real parameters in 2D (resp. 3D) systems. These $d(2\,d + 1)$ free real parameters physically correspond to the existence of exactly $d(2\,d + 1)$ independent scattering channels as we demonstrate below (see Fig. 3 for the 2D case). Note that the set of unitary symmetric matrices forms a group which is isomorphic to the symplectic group. In Appendix A, we show how this set of scattering matrices is related to the usual set of transfer matrices.

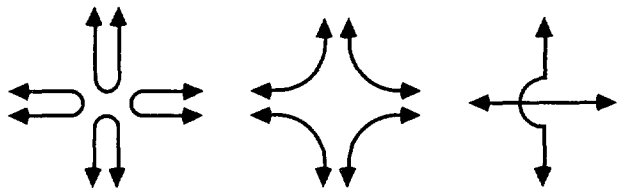

Fig. 3. — Sketch of the 10 elementary scattering processes described by the S-matrix : 2 transmissions, 4 $\pi/2$-scattering events and 4 reflections.

The 2d by 2d unitary and symmetric S-matrices can be parametrized under the form

$$S = \begin{bmatrix} L & M \\ {}^tM & L' \end{bmatrix} \tag{4}$$

with

$$L = -\,{}^tV \cos\delta\, V \quad ({}^tV \text{ means transposed of } V) \tag{5a}$$

$$L' = U \cos\delta\, {}^tU \tag{5b}$$

$$M = U \sin\delta\, V \tag{5c}$$

U and V are arbitrary unitary d by d matrices parametrised by $2\,d^2$ reals and

$$\cos\delta = \begin{bmatrix} \cos\delta_1 & & 0 \\ & \cdot & \\ 0 & & \cos\delta_d \end{bmatrix}, \quad \sin\delta = \begin{bmatrix} \sin\delta_1 & & 0 \\ & \cdot & \\ 0 & & \sin\delta_d \end{bmatrix} \tag{6}$$

are d by d diagonal matrices.

2.2 THE TWO-DIMENSIONAL CASE. — In two dimensions ($d = 2$), the S-matrix is thus defined by the following expression, where the four fields E_i, $i = 1$ to 4 impinging upon the scatterer

along its four links are transformed into four outgoing fields O_i, $i = 1$ to 4 as depicted in figure 2a :

$$\begin{pmatrix} O_1 \\ O_2 \\ O_3 \\ O_4 \end{pmatrix} = (S) \begin{pmatrix} E_1 \\ E_2 \\ E_3 \\ E_4 \end{pmatrix}. \tag{7}$$

Ten real parameters are then required to characterize completely a 4 by 4 S-matrix. The condition that S be symmetric reduces to 10 complex parameters and the condition of unitarity to 10 real parameters. An appropriate parametrization for arbitrary unitary 2 by 2 matrices is

$$V = e^{i\alpha} \begin{bmatrix} 1 & 0 \\ 0 & i\, e^{i\rho} \end{bmatrix} \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} e^{i\gamma} & 0 \\ 0 & e^{-i\gamma} \end{bmatrix} \tag{8a}$$

$$U = e^{i\alpha'} \begin{bmatrix} 1 & 0 \\ 0 & i\, e^{i\rho'} \end{bmatrix} \begin{bmatrix} \cos\theta' & -\sin\theta' \\ \sin\theta' & \cos\theta' \end{bmatrix} \begin{bmatrix} e^{i\gamma'} & 0 \\ 0 & e^{-i\gamma'} \end{bmatrix} \tag{8b}$$

where α, ρ, θ, γ, α', ρ', θ' and γ' are real numbers generally chosen in the interval $[0, 2\pi]$. Noting

$$\cos\delta = \begin{bmatrix} \cos\delta_1 & 0 \\ 0 & \cos\delta_2 \end{bmatrix}, \qquad \sin\delta = \begin{bmatrix} \sin\delta_1 & 0 \\ 0 & \sin\delta_2 \end{bmatrix} \tag{9}$$

we obtain by inserting expressions (6) and (7) into (5) :

$$L = -e^{2i\alpha} \begin{cases} e^{2i\gamma}[\cos\delta_1 \cos^2\theta - \cos\delta_2 \sin^2\theta\, e^{2i\rho}] & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ + e^{-2i\gamma}[\cos\delta_1 \sin^2\theta - \cos\delta_2 \cos^2\theta\, e^{2i\rho}] & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ - [\cos\delta_1 + \cos\delta_2 e^{2i\rho}] \sin\theta \cos\theta & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{cases} \tag{10a}$$

$$L' = +e^{2i\alpha} \begin{cases} e^{2i\gamma'}[\cos\delta_1 \cos^2\theta' - \cos\delta_2 \sin^2\theta'\, e^{2i\rho'}] & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ + e^{-2i\gamma'}[\cos\delta_1 \sin^2\theta' - \cos\delta_2 \cos^2\theta'\, e^{2i\rho}] & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ - [\cos\delta_1 + \cos\delta_2 e^{2i\rho'}] \sin\theta' \cos\theta' & \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{cases} \tag{10b}$$

$$M = -e^{i(\alpha+\alpha')} \times$$

$$\times \begin{cases} e^{i(\gamma+\gamma')}[\sin\delta_1 \cos\theta \cos\theta' - \sin\delta_2 \sin\theta \sin\theta' e^{i(\rho+\rho')}] & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ + e^{-i(\gamma+\gamma')}[\sin\delta_1 \sin\theta \sin\theta' - \sin\delta_2 \cos\theta \cos\theta' e^{i(\rho+\rho')}] & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ - e^{i(\gamma-\gamma')}[\sin\delta_1 \cos\theta \sin\theta' + \sin\delta_2 \sin\theta \cos\theta' e^{i(\rho+\rho')}] & \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ - e^{-i(\gamma-\gamma')}[\sin\delta_1 \sin\theta \cos\theta' + \sin\delta_2 \cos\theta \sin\theta' e^{i(\rho+\rho')}] & \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \end{cases} \tag{10c}$$

An intuitive way to understand this parametrization is to consider the four links around a node, along the four cardinal directions : east (E), west (W), north (N) and south (S). A wave coming from the south for example is redirected in all directions after scattering : it is partly reflected back to the south, partly transmitted to the north, while part of it makes a left turn to west, the rest turning right to east. In this representation, the scattering of a wave impinging on the four links of a node decomposes itself into ten elementary transfer events : four reflections ($E \leftrightarrow E$, $W \leftrightarrow W$, $S \leftrightarrow S$, $N \leftrightarrow N$) represented by the 4 elementary matrices

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix};$$

two transmissions ($E \leftrightarrow W$, $S \leftrightarrow N$) represented by the 2 elementary matrices

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix};$$

and four $\pi/2$ rotations ($E \leftrightarrow N$, $W \leftrightarrow S$, $N \leftrightarrow W$, $S \leftrightarrow E$)

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

This shows geometrically the origin of the ten parameters α, ρ, θ, γ, α', ρ', θ', γ', δ_1 and δ_2 (see also Fig. 3), which are just enough and sufficient to control the relative weight of the ten elementary scattering processes. This reasoning is straightforwardly generalized to other dimensions and justifies the geometrical interpretation of the existence of the $d(2d+1)$ free real parameters defining the unitary symmetric S-matrices.

Keeping these parameters arbitrary corresponds to describing general anisotropic media. It will be convenient below to restrict our attention to isotropic scatterers. In this case, the ten real parameters can be reduced to three real parameters. Indeed, isotropy implies that the two transmissions and the four reflections are equivalent, which sets $\alpha' = \alpha + \pi/2$, $\gamma = \gamma'$, $\rho = \rho'$ and $\theta = \theta'$. It also implies that the four rotations are equivalent which yields discrete sets of choices for the parameters δ_2 (ou δ_1), γ and θ. Appendix B gives a list of the different sets of parameters allowed for the parametrization of isotropic S-matrices, i.e. which verify $L = L'$, $M = M'$ and $M_{11} = M_{22} = M_{12} = M_{21}$.

In the following we have chosen one set of parameters $\delta_2 = 0$, $\gamma = 0$ and $\theta = -\pi/4$ which gives

$$L = L' = -\frac{1}{2} e^{2i\alpha} \left[(\cos \delta_1 - e^{2i\rho}) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + (\cos \delta_1 + e^{2i\rho}) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right] \tag{11a}$$

$$M = \frac{i}{2} e^{2i\alpha} \left[\sin \delta_1 \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \right]. \tag{11b}$$

The three real parameters α, δ_1 and ρ control the phase acquired by the scattered waves and the strength of the scattering process. For instance when $\delta_1 \equiv \delta = \pi$, the matrix M is zero and only the transmission and reflection processes are left. Setting ρ to 0 removes the second term in L, corresponding to the transmission contribution. In this case $\delta_1 \equiv \delta = \pi$ and

$\rho = 0$, the only processes to take place are reflections back and forth between two neighboring nodes : the system is then reduced to a series of independent uncoupled channels where the wave is captured, remisniscent of localized orbitals in the tight-binding model of electrons in dirty metals [28]. When having in mind the Anderson localization phenomenon, this limit is particularly interesting since it corresponds to a trivial on-site localization. In the spirit of the locator expansion pioneered by Anderson [29], any perturbation around this choice of parameters $\delta_1 \equiv \delta = \pi$ and $\rho = 0$ will weakly couple the localized channels. The localization problem then reduces to the study of the effect of the weak coupling between localized orbitals. Of course, this limit is also interesting from the numerical point of view since we expect the localization length to become very small close to this limit.

In the following, we then keep the parameter ρ set to 0 while δ and α stay free parameters. The 2 by 2 matrices L, L' and M entering the definition of the S-matrix are now simply parametrized under the form

$$L = L' = e^{2i\alpha}\left[-\sin^2 \delta/2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \cos^2 \delta/2 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right] = r\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + t\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad (12a)$$

$$M = i\, e^{2i\alpha}\left[\sin \delta/2 \cos \delta/2 \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\right] = d\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \quad (12b)$$

$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ represents the reflection terms, $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ the transmission terms and $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ the rotation terms. r (resp. t) is the amplitude reflection (resp. transmission) coefficient and d is the amplitude coefficient of the four $\pi/2$ scattering events. The parameter δ is a measure of the scattering strength and α is a measure of the phase shift acquired by the wave at each encounter with the scatterer. Figure 4 depicts the dependence of $|t|$, $|r|$ and $|d|$ as a function of δ. It is sufficient to choose the parameter δ in the interval $[0, \pi]$. For $\delta = 0$, the S-matrix is transparent and the wave crosses over the node keeping the same direction while taking a phase shift equal to 2α. This is the 1D-limit since the 2D lattice can then be considered as a set of independent horizontal and vertical lines on which waves propagate without distorsions. At the other extreme $\delta = \pi$, the reflection coefficient is equal to $-e^{2i\alpha}$ and is of unit modulus whereas all other processes disappear. The node possessing such an S-matrix is perfectly

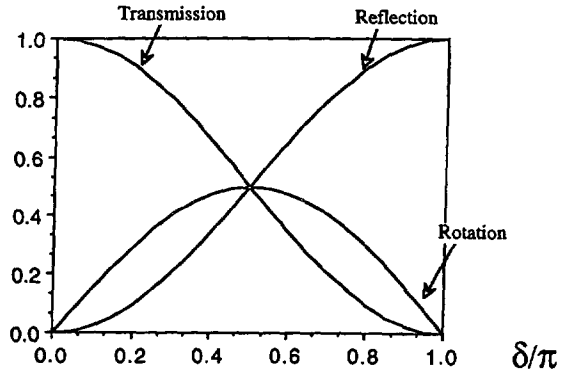

Fig. 4. — Dependence of the modulus $|r| = \sin^2 \delta/2$ of reflection term, the transmission term $|t| = \cos^2 \delta/2$ and the $\pi/2$-rotation term $|d| = \sin \delta/2 \cos \delta/2$ as a function of the scattering strength parameter δ, in the parametrization given by equation (12).

reflecting. Varying δ between 0 and π then allows one to weight continuously the strength of the three scattering processes (transmission, reflection and $\pi/2$ scattering).

The meaning of the parameter δ is best illustrated by calculating the elastic σ_e and transport σ_t scattering « cross sections » of such an S-matrix. σ_e is the sum of all scattering intensities off the initial direction. This yields

$$\sigma_e = 1 - |t|^2 = 1 - \cos^4 \delta/2 . \tag{13}$$

The transport scattering cross section is similarly defined but with a weight $(1 - \cos \mathbf{i} \cdot \mathbf{s})$ multiplying each term, where $\mathbf{i}$ (resp. $\mathbf{s}$) is the unit vector in the incident (resp. scattered) direction. We thus obtain

$$\sigma_t = 2 \sin^2 \delta/2 . \tag{14}$$

Note that we recover $\sigma_e = \sigma_t = 0$ for $\delta = 0$ and $\sigma_e = 1$ and $\sigma_t = 2$ for $\delta = \pi$. Recall that these scattering cross sections are written in the units where the lattice size is unity.

A given system will then be defined by the set of 4 by 4 unitary symmetric S-matrices parametrized using equations (5) and (12), with one S-matrix per node. The case where all the S-matrices are the same on all nodes corresponds to a periodic system. A quenched random system is defined by a set of S-matrices, one for each node, with random choices for the real parameters α and δ. We can also choose to take the same δ for all matrices and take random choices for α. The latter model has the advantage that all S-matrices have the same scattering efficiency (same scattering cross sections) and differ only by the phase shift taken by a scattered wave. This has the advantage of putting the emphasis on the wave phase, which might turn out to be useful in the future in order to study Anderson wave localization, a phenomenon deeply associated with phase coherence. This is the choice that has been made in most of our computation [21]. The parameters of the model for a given random system used in the companion paper [21] are the scattering strength δ of the S-matrices and the width $\Delta\alpha$ in which the random phase α is randomly chosen from one node to another : $\alpha \in [-\Delta\alpha ; +\Delta\alpha]$.

Note that there are in total $4 L^2$ modes in a system of size L by L, since there are 2 bonds per node and 2 directions of propagation (i.e. degrees of freedom) per bond. A degenerate case which is straightforward to check occurs when $\delta = \pi$, such as all bonds become independent from each other. However, it is simpler and more transparent to deal with only one of the two sublattices. This restricts the number of mode to $2 L^2$.

2.3 PHYSICAL CONTENT OF THE WAVE AUTOMATON AND ADVANTAGES. — It is physically illuminating to give a direct derivation of the structure of the S-matrix in the isotropic case. As shown in figure 5a, we consider a pulse wave of amplitude 1 incident upon an isotropic scatterer. An amplitude t (resp. r and d) is transmitted (resp. reflected and scattered at an angle $\pi/2$). The condition of time reversal invariance is that the time reverse scattering event, consisting of four incident fields of amplitudes r^*, t^*, d^* and d^* (see Fig. 5b), leads to an outgoing wave of amplitude 1 on the link on which the initial pulse was incident and to no waves on the other links. This yields the three real equations :

$$|t|^2 + |r|^2 + 2\,|d|^2 = 1 \tag{15a}$$

$$r t^* + r^* t + 2\,|d|^2 = 0 \tag{15b}$$

$$(r + t)\, d^* + (r^* + t^*)\, d = 0 . \tag{15c}$$

These conditions which signify that the S-matrix is unitary and symmetric are of course satisfied by the choice of parameters (10) or (12). It is clear that conditions (15) and especially

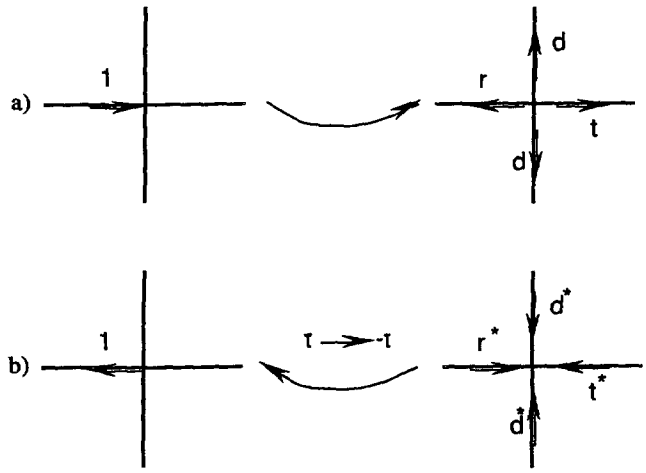

Fig. 5. — Definition of the scattering amplitude in the isotropic case and illustration of the time reversal invariance condition : a) direct scattering event ; b) time reverse scattering event.

the time reversal invariance (15b-c) lead to strong constraints on the form of the S-matrix. To illustrate this point physically, let us consider the example of a laser beam separated into two beams by a semi-reflective miror (such that only t and d are non-vanishing) and then recombined later to give two other beams (see Fig. 6). If we just allow for the conservation of energy for this interaction with the semi-reflective mirors, we could imagine that $t = d = 1/\sqrt{2}$ is a suitable choice since the energy $|t|^2 + |d|^2 = 1$ is conserved. However, upon the recombining process at the other end of the system, we recover a total energy which is twice the value that has been put in at the beginning. Note that the recombining process acts in a way similar to the time reverse scattering process shown in figure 5. The solution to this problem is for example found by taking $t = 1/\sqrt{2}$ and $d = i/\sqrt{2}$, i.e. allowing for a $\pi/2$ phase shift between the waves transmitted and reflected by the semi-reflective miror. More generally, when dealing with scattering processes in which a wave is incident on several channels, it is important to choose the S-matrix, i.e. the scattering amplitudes t, r and d such that (15) is verified, in the isotropic case.

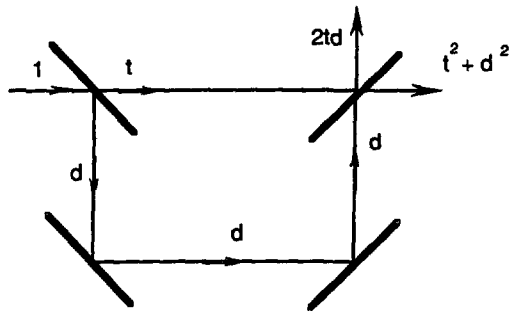

Fig. 6. — Example of a laser beam separated into two beams by a semi-reflective miror (such that only t and d are non-vanishing) and then recombined later to give two other beams. If $t = d = 1/\sqrt{2}$, the total outgoing energy $|2\,td|^2 + |t^2 + d^2|^2 = 2$ is twice the injected energy ! This paradox is solved by the choice $t = 1/\sqrt{2}$ and $d = i/\sqrt{2}$, meaning that the phase difference between t and d is not arbitrary.

3. Periodic systems.

Periodic systems are constructed by taking the same S-matrix on all L^2 nodes of the lattice. In the simple case that we consider, namely that the same δ is chosen for all matrices, the periodic case corresponds to taking the same α on all sites. As we now show, the study of periodic systems is useful to better understand the status of the wave automaton model. It will also be useful for the more general case of a random system studied in [21], since the interaction of a Bloch wave with a single impurity (corresponding to a different S-matrix on one node in a « sea » of identical S-matrices) can be calculated analytically, and allows us to derive the elastic mean free time τ_e and mean free length ℓ_e as a function of the model parameters and the frequency $f = \omega/2\pi$. In turn, the elastic mean free time τ_e is the key parameter entering the weak localization predictions which will be tested with our numerical calculations in [21].

Let us consider the Bloch wave propagating in the direction **k** at pulsation ω, on one of the two square sublattices of size L by L, and containing n^2 nodes with $n = L/\sqrt{2}$. Let us denote it by a vector $\mathbf{A}(\mathbf{k}, \tau)$ whose $4n^2$ components (n^2 nodes with 4 incident fields per node) read

$$A_m^{(i,j)}(\tau) = a_m \, e^{i(\omega\tau - k_x i - k_y j)} \qquad i, j = 1, n, \quad m = 1, 4 \tag{16}$$

$A_m^{(i,j)}(\tau)$ denotes the amplitude of the scalar field impinging on node (i, j) at time τ in the direction of the bond m (we use the index notation given in Fig. 1). k_x and k_y are the two components of the Bloch wave vector **k**.

Let us recall that the structure of the square lattice and the definitions of our wave automaton imply that the wave propagation can be considered as the superposition of a wave propagation on two independent sublattices. To make this point clear, consider a wave impinging on node (i, j) at time τ. This wave is scattered in all four directions and reaches the nodes $(i+1, j)$, $(i, j+1)$, $(i-1, j)$ and $(i, j-1)$ at time $\tau + 1$. It is only at time $\tau + 2$ that the wave is scattered back on the original node (i, j) as well as on the next nearest neighboring nodes. Consequently, each node is visited every two time steps which means that the square lattice can be seen as the superposition of two independent sublattices, each one being visited by the wave every two time steps (see Fig. 1). Since the wave is defined on the same sublattice only at time τ and $\tau + 2p$ (where p is an integer), the scattering event at $\tau + (2p+1)$ is an intermediate step on the other sublattice. This lets us free to choose an additional phase 0 or π at each time step since the relevant phase shift is $e^{2i\omega}$. This implies that expression (16) can be generalized by multiplication by a factor ± 1. Accordingly, the expression of the Bloch wave can be either (16) or the following expression

$$A_m^{(i,j)}(\tau) = e^{i\pi\tau} \, a_m \, e^{i(\omega\tau - k_x i - k_y j)} \qquad i, j = 1, n, \quad m = 1, 4 \tag{17}$$

where $e^{i\pi\tau}$ represents this additional phase. This would no longer be true on a triangular or hexagonal lattice, for instance. In the case of the triangular lattice, the S-matrices must be 6 by 6, corresponding to 21 free real parameter and for hexagonal lattice the S-matrices must be 3 by 3, corresponding to 6 free real parameters. Thus, in addition to the square lattice for arbitrary anisotropic S-matrices, such lattices offer the possibility of modelling different types of anisotropic media. They will not be considered below.

As a result of this self-dual property of the square geometry, if the local incident field $\Psi_{i,j}^{\text{in}}(\tau)$ at node (i, j) at time τ has the four components :

$$\Psi_{i,j}^{\text{in}}(\tau) = \left\{A_1^{(i,j)}(\tau), A_2^{(i,j)}(\tau), A_3^{(i,j)}(\tau), A_4^{(i,j)}(\tau)\right\},$$

the resulting local output field $\Psi_{i,j}^{\text{out}}(\tau + 1)$ at time $\tau + 1$ after a scattering event at node (i, j), will be either

$$\Psi_{i,j}^{\text{out}}(\tau + 1) = \left\{A_2^{(i,j-1)}(\tau + 1),\ A_1^{(i,j+1)}(\tau + 1),\ A_4^{(i-1,j)}(\tau + 1),\ A_3^{(i+1,j)}(\tau + 1)\right\}$$

or

$$\Psi_{i,j}^{\text{out}}(\tau + 1) = \left\{-A_2^{(i,j-1)}(\tau + 1),\ -A_1^{(i,j+1)}(\tau + 1),\ -A_4^{(i-1,j)}(\tau + 1),\ -A_3^{(i+1,j)}(\tau + 1)\right\}.$$

Inserting these two expressions in the scattering equation at node (i, j):

$$\Psi_{i,j}^{\text{out}}(\tau + 1) = S\Psi_{i,j}^{\text{in}}(\tau)$$

provides two systems of four homogeneous equations. These systems have non-zero solutions if their determinant is zero which provides the following dispersion relations :

$$(\cos(\omega - 2\alpha) - \cos k_x)(\cos(\omega - 2\alpha) - \cos k_y) = \sin^2(\omega - 2\alpha)\,\mathrm{tg}^2\,\delta/2 \tag{18}$$

$$(\cos(\omega - 2\alpha) + \cos k_x)(\cos(\omega - 2\alpha) + \cos k_y) = \sin^2(\omega - 2\alpha)\,\mathrm{tg}^2\,\delta/2\,. \tag{19}$$

Each of these relations yields two branches for the dispersion equation in the first Brillouin zone ($k_x, k_y \in [0, \pi]$ and $\omega \in [0, \pi/2]$), $\omega_1(k_x, k_y)$ and $\omega_2(k_x, k_y)$ for equation (18), $\omega_3(k_x, k_y)$ and $\omega_4(k_x, k_y)$ for equation (19) :

$$\omega_1(k_x, k_y) = 2\alpha + \mathrm{Arcos}\left\{\cos\delta/2\cos(k_x + k_y)/2\right\} + \mathrm{Arcos}\left\{\cos\delta/2\cos(k_x - k_y)/2\right\} \tag{20a}$$

$$\omega_2(k_x, k_y) = 2\alpha + \mathrm{Arcos}\left\{\cos\delta/2\cos(k_x + k_y)/2\right\} - \mathrm{Arcos}\left\{\cos\delta/2\cos(k_x - k_y)/2\right\} \tag{20b}$$

$$\omega_3(k_x, k_y) = 2\alpha + \pi - [\mathrm{Arcos}\left\{\cos\delta/2\cos(k_x + k_y)/2\right\} - \mathrm{Arcos}\left\{\cos\delta/2\cos(k_x - k_y)/2\right\}] \tag{21a}$$

$$\omega_4(k_x, k_y) = 2\alpha + \pi - [\mathrm{Arcos}\left\{\cos\delta/2\cos(k_x + k_y)/2\right\} + \mathrm{Arcos}\left\{\cos\delta/2\cos(k_x - k_y)/2\right\}]\,. \tag{21b}$$

Note that a non-vanishing scattering phase α has the simple effect of just shifting ω (for the same k_x and k_y), resulting in a possible overlap and folding between adjacent Brillouin zones. There is thus no loss of generality by posing $\alpha = 0$ in the periodic case. Then, $\omega \in [0, \pi/2]$. The dispersion relation $\omega(k_x, k_y)$ deduced from equation (20) is represented in figure 7 for different values of δ.

Two regimes are found :

1) when $\delta > \pi/2$, a gap appears in the structure for $\omega \in [\pi - \delta, \pi/2]$;
2) when $\delta \leqslant \pi/2$, this gap disappears and the two branches overlap.

The density of state $g(\omega) = \int \mathrm{d}k_x \int \mathrm{d}k_y\,|\nabla_{\mathbf{k}}\omega|^{-1}$ giving the number of eigenmodes with pulsations between ω and $\omega + \mathrm{d}\omega$, is shown in figure 8, for different values of parameter δ. For $\delta = 0.7\,\pi$, the gap extends from $\omega = 0.3\,\pi$ to $0.5\,\pi$ and $g(\omega) = 0$ in this interval. For $\delta = 0.3\,\pi$, $g(\omega)$ is constant in the same interval $\omega \in [0.3\,\pi, 0.5\,\pi]$, as a consequence of the overlap of the two symmetric branches (20a) and (20b) of the dispersion relation.

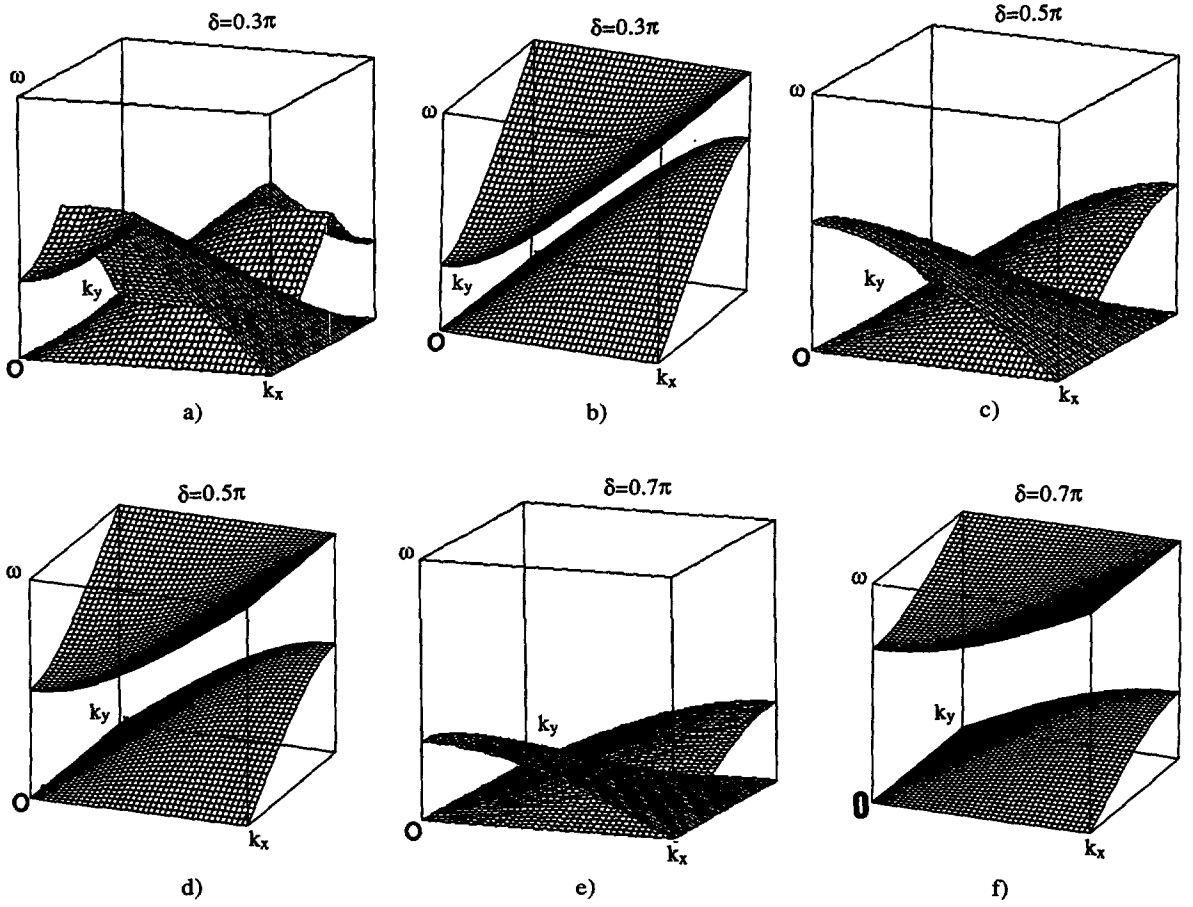

Fig. 7. — Dispersion relation $\omega(k_x, k_y)$: the z-axis corresponds to $0 \leq \omega \leq \pi$, the x-axis (resp. y-axis) corresponds to $0 \leq k_x \leq \pi$ (resp. $0 \leq k_y \leq \pi$). a) Dispersion relation for $\delta = 0.3\ \pi$ and for the time-dynamic version computed every two time steps corresponding to the analysis of one of the two square sub-lattices. In this case, $0 \leq \omega \leq \pi/2$; b) same as a) but for the calculation every time step, which is a superposition of the two decoupled problems on the two sublattices (see text). In this case, $0 \leq \omega \leq \pi$. Note that figure 7b is deduced from figure 7a by simple symmetry operations. This figure shows the absence of gap. c) Dispersion relation for $\delta = 0.5\ \pi$ and for the time-dynamic version computed every two time steps corresponding to the analysis of one of the two square sub-lattices. In this case, $0 \leq \omega \leq \pi/2$; d) same as c) but for the calculation every time step, which is a superposition of the two decoupled problems on the two sublattices (see text). In this case, $0 \leq \omega \leq \pi$. This value $\delta = 0.5\ \pi$ is marginal and the gap begins to open for $\delta > 0.5\ \pi$. e) Dispersion relation for $\delta = 0.7\ \pi$ and for the time-dynamic version computed every two time steps corresponding to the analysis of one of the two square sub-lattice. In this case, $0 \leq \omega \leq \pi/2$; f) same as e) but for the calculation every time step, which is a superposition of the two decoupled problems on the two sublattices (see text). In this case, $0 \leq \omega \leq \pi$. The presence of the gap is clearly apparent.

These analyse reveal the nature of the physics embedded in the parametrization of the S-matrices in terms of α and δ. It turns out that this parametrization makes the wave automaton analogous to a time-dependent tight-binding model [28] with additional second-nearest neighbor coupling. The analogy is best seen by looking at figure 9. Let us divide the initial

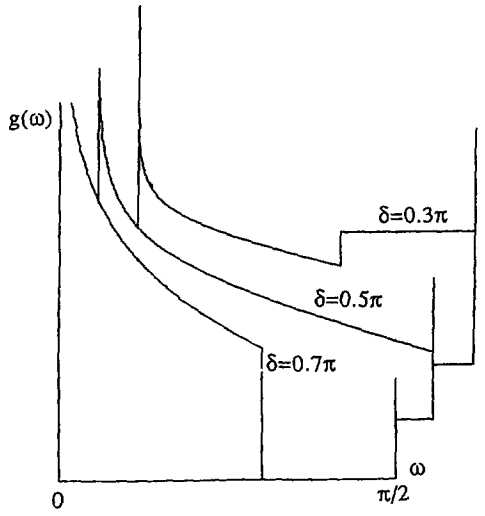

Fig. 8.

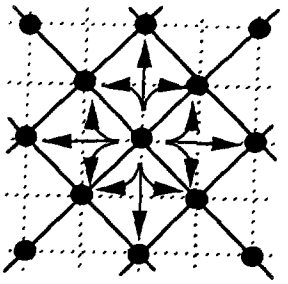

Fig. 9.

Fig. 8. — Representation of the density of states $g(\omega)$ (in the same arbitrary units) for $\delta = 0.3\ \pi$, $\delta = 0.5\ \pi$ and $\delta = 0.7\ \pi$.

Fig. 9. — Connection between the « wave automaton » and the tight-binding model (see text). The original lattice is represented by dotted lines. The sub-lattice coined « 1 », on which the tight-binding model is defined, is represented by the full lines and the black dots. The 4 $\pi/2$-scattering processes of the intermediate node of lattice « 2 » connect the site (i, j) of lattice « 1 » to its four nearest neighbors, the 4 transmissions connect (i, j) to its four second nearest neighbors along the diagonals and the 4 reflections control the on-site term.

square lattice into two interpenetrating square sub-lattices orientated at 45°. We choose one of these sub-lattices (coined « 1 » hereafter and represented by the black dots in Fig. 9) as being that on which the tight-binding model will be defined. We attribute a wave intensity to each node of « 1 » equal to the sum of the intensities of its four outgoing waves just after a scattering event. One can then show that these four outgoing waves on each node of « 1 » at time t reach at time $t + 2$ its four nearest neighbors, its four second nearest neighbors along the diagonal and are partially reflected to the initial node. If we look at the wave field every two time steps, we can forget the other sub-lattice « 2 » except that it provides the intermediate scattering step. We thus obtain a version of the tight-binding model for an electron in a random potential, with diagonal second nearest neighbor coupling. The four $\pi/2$ scattering processes of the intermediate node of lattice 2 provide the coupling to the four nearest neighbours, the two transmissions provide the coupling with the four second nearest neighbours along the diagonals and the four reflections control the on-site term. The relative strength of the on-site potential to the hopping terms is controlled by the parameter δ, as shown in figure 4. Note that in the limit $\delta = \pi$, the wave on each bond oscillates back and forth between its two extremities, in a way completely similar to a bound isolated orbital. When δ decreases from π, these localized orbitals become coupled *via* nearest neighbor and next-nearest neighbor « hopping » terms.

The structure of the dispersion relation in the limit of small k_x and k_y (or small $\pi - k_x$ and $\pi - k_x$ which is the other Brillouin border) in a periodic array of S-matrices allows us to characterize further the parametrization in terms of α and δ. Expressions (20) and (21)

yield

$$\omega_1(k_x, k_y) = 2\,\alpha + \frac{k_x\,k_y}{2\tan\delta/2} \tag{22a}$$

$$\omega_2(k_x, k_y) = 2\,\alpha + \frac{k_x^2 + k_y^2}{4\tan\delta/2} \tag{22b}$$

$$\omega_3(k_x, k_y) = 2\,\alpha + \pi - \delta - \frac{k_x^2 + k_y^2}{4\tan\delta/2} \tag{23a}$$

$$\omega_4(k_x, k_y) = 2\,\alpha + \pi - \frac{k_x\,k_y}{2\tan\delta/2}\,. \tag{23b}$$

The quadratic dispersion relations (22b) and (23a) for $\omega_2(k_x, k_y)$ and $\omega_3(k_x, k_y)$ are typical of the tight-binding model for small k (quadratic dispersion relation). The analog of the hopping coefficient is thus given by $1/[4\tan\delta/2]$. Moreover, the other branches $\omega_1(k_x, k_y)$ and $\omega_4(k_x, k_y)$ reveal the specificity of our chosen parametrization in term of α and δ. In the infrared limit (k_x and $k_y \ll 1$), ω_1 is still quadratic but a fixed k_x or k_y, it goes to $2\,\alpha$ *linearly* in k_y or k_x. This branch has also the special feature that ω_1 can come close to $2\,\alpha$ (i.e. the product $k_x\,k_y$ goes to zero) while either k_x or k_y remain arbitrarily large (as long as the product remains small).

The Bloch modes $A_m^{(l,J)}(\tau)$ are easily calculated from the scattering equation. Indeed, if the determinant of the homogeneous system is zero, the homogeneous solution is such that three of the amplitudes (say a_2, a_3, a_4) can be expressed as a function of one of them (say a_1) :

$$a_2 = a_1\,e^{-ik_x}\,\frac{\sin\left(\dfrac{\omega - k_y}{2}\right)}{\sin\left(\dfrac{\omega + k_y}{2}\right)} \tag{24a}$$

$$a_3 = -\,a_1\,e^{-i\left(\frac{k_x - k_y}{2}\right)}\,\frac{\sin\left(\dfrac{\omega + k_x}{2}\right)}{\sin\left(\dfrac{\omega + k_y}{2}\right)}\,\frac{\cos(\omega - \delta/2) - \cos k_y\cos\delta/2}{\cos(\omega - \delta/2) - \cos k_x\cos\delta/2} \tag{24b}$$

$$a_4 = -\,a_1\,e^{-i\left(\frac{k_x - k_y}{2}\right)}\,\frac{\sin\left(\dfrac{\omega - k_x}{2}\right)}{\sin\left(\dfrac{\omega + k_y}{2}\right)}\,\frac{\cos(\omega - \delta/2) - \cos k_y\cos\delta/2}{\cos(\omega - \delta/2) - \cos k_x\cos\delta/2}\,. \tag{24c}$$

Note that for $\alpha \neq 0$, it suffices to replace ω by $\omega - 2\,\alpha$ or $\omega - 2\,\alpha - \pi$ to get the general expressions. Because the Bloch modes form a basis in the mode space, the normalisation $\left\langle \Psi^{\text{in}}_{l',J'}(\tau),\ \Psi^{*\,\text{in}}_{l,J}(\tau)\right\rangle = \delta_{(l',J'),(l,J)}$ is required and yields a fourth relation between the amplitudes a_1, a_2, a_3, a_4 .

$$|a_1|^2 + |a_2|^2 + |a_3|^2 + |a_4|^2 = 1\,. \tag{25}$$

We finally obtain the expressions of the Bloch modes as

$$a_1 = \frac{1}{\sqrt{D}}\sin\left(\frac{\omega + k_y}{2}\right)(\cos(\omega - \delta/2) - \cos k_x\cos\delta/2)\,e^{ik_x/2} \tag{26a}$$

$$a_2 = \frac{1}{\sqrt{D}} \sin\left(\frac{\omega - k_y}{2}\right) (\cos(\omega - \delta/2) - \cos k_x \cos \delta/2)\, e^{-ik_x/2} \tag{26b}$$

$$a_3 = -\frac{1}{\sqrt{D}} \sin\left(\frac{\omega + k_x}{2}\right) (\cos(\omega - \delta/2) - \cos k_y \cos \delta/2)\, e^{ik_y/2} \tag{26c}$$

$$a_4 = -\frac{1}{\sqrt{D}} \sin\left(\frac{\omega - k_x}{2}\right) (\cos(\omega - \delta/2) - \cos k_y \cos \delta/2)\, e^{-ik_y/2} \tag{26d}$$

where

$$D = (1 - \cos\omega \cos k_y)(\cos(\omega - \delta/2) - \cos k_x \cos \delta/2)^2 + \\ + (1 - \cos\omega \cos k_x)(\cos(\omega - \delta/2) - \cos k_y \cos \delta/2)^2 \tag{27}$$

These expressions are used in the following paper [21] to analyze the interaction of a Bloch wave with a defect.

4. Conclusions.

We have described in detail a new lattice model, the « wave automaton » for the *dynamical* propagation of waves in arbitrary heterogeneous media. It treats the field as a continuous complex number and the time and space are discrete. This model does not belong to the class of cellular automata but is rather analogous to so-called coupled maps, used to model spatio-temporal chaotic systems. We thus use the term « automaton » in the broader pre- von Neumann sense of an artificial « creature » (here the complex field) imitating real life (the wave), and not in the restricted meaning of a Boolean or discrete variable. In the companion paper [21], we show that it is efficient for calculations on large systems (1 024 × 1 024) over long times (several 10^6 inverse band widths). We have detailed the construction of the wave automaton, and in particular the parametrization of the S-matrix on each node of the lattice. We have given the analytical form of the dispersion relation, density of states and Bloch modes for periodic systems. This understanding is useful in order to be able to model a variety of systems. In the companion paper [21], we use the wave automaton to analyze quantitatively the time evolution of the spreading of a wave packet in a 2D disordered system.

In a work in preparation, we will explore another class of parameters for the wave automaton, such that the continuous limit of the model yields the hyperbolic wave equation and the Klein-Gordon equation. Taking time reversal invariance breakdown (due to the presence of a magnetic field for instance) into account, loss, gain and various types of nonlinearities are also possible and are under active study.

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Appendix A.

Relation between the scattering matrix (S-matrix) representation and the usual transfer matrix (T-matrix) representation :

T-matrix (see Fig. 1) :

$$\begin{pmatrix} E_2 \\ S_1 \end{pmatrix} = T \begin{pmatrix} S_2 \\ E_1 \end{pmatrix}$$

with $$T = \begin{pmatrix} \alpha & \beta \\ \alpha^* & \beta^* \end{pmatrix} \quad \text{(symmetry condition)}$$

$$\alpha\alpha^{*t} - \beta\beta^{*t} = 1 \quad \text{and} \quad \alpha\beta^t = \beta^t\alpha \quad \text{(unitarity condition)}.$$

S-matrix :

$$\begin{pmatrix} S_2 \\ S_1 \end{pmatrix} = S \begin{pmatrix} E_1 \\ E_2 \end{pmatrix}$$

with $$S = \begin{pmatrix} L & M \\ M' & L' \end{pmatrix}$$

r, r', t and t' are related to α and β by the relations :

$$L = -(\alpha^*)^{-1}\beta^*$$
$$L' = \beta(\alpha^*)^{-1}$$
$$M = (\alpha^{*t})^{-1}$$
$$M' = M^t.$$

Appendix B.

List of the different sets of parameters possible for the parametrization of S-matrix that describes isotropic scattering, that is to say, with $L = L'$, $M = M'$ and $M_{11} = M_{22} = M_{12} = M_{21}$. Essentially, the first condition gives two branches : either $\rho = \rho' + \pi/2$, $\gamma = \gamma'$, $\theta = \theta'$, $\alpha = \alpha'$ and $\cos\delta_1 = 0$, or $\alpha = \alpha' + \pi/2$, $\gamma = \gamma'$ and $\rho = \rho'$; then, condition $M_{12} = M_{21}$ gives $\gamma = 0$ or $\gamma = \pi/2$; finally, $M_{11} = M_{22}$ sets a choice either for θ or for δ_1 (resp. δ_2) and $M_{11} = M_{12}$ reduces again to three or two the number of free parameters.

$$1\,a - \left\{ \begin{array}{c} \rho = \rho' \pm \pi/2 \\ \gamma = \gamma' = 0 \\ \alpha = \alpha' \\ \delta_1 = +\pi/2 \\ \theta = -\pi/4 \text{ or } 3\pi/4 \\ \delta_2 = 0 \end{array} \right\} \quad \text{and} \quad \left\{ \begin{array}{c} \rho = \rho' \pm \pi/2 \\ \gamma = \gamma' = \pi/2 \\ \alpha = \alpha' \\ \delta_1 = -\pi/2 \\ \theta = +\pi/4 \text{ or } -3\pi/4 \\ \delta_2 = \pi \end{array} \right\}$$

$$\text{gives} \left\{ \begin{array}{c} L = +\frac{1}{2} e^{2i(\alpha+\rho)} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \\ \text{and} \\ M = +\frac{1}{2} e^{2i\alpha} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{array} \right\}$$

$$1\,b - \begin{pmatrix} \rho = \rho' \pm \pi/2 \\ \gamma = \gamma' = 0 \\ \alpha = \alpha' \\ \delta_1 = \pi/2 \\ \theta = -\pi/4 \text{ or } 3\,\pi/4 \\ \delta_2 = \pi \end{pmatrix} \text{ and } \begin{pmatrix} \rho = \rho' \pm \pi/2 \\ \gamma = \gamma' = \pi/2 \\ \alpha = \alpha' \\ \delta_1 = -\pi/2 \\ \theta = +\pi/4 \text{ or } -3\,\pi/4 \\ \delta_2 = 0 \end{pmatrix}$$

$$\text{gives} \begin{pmatrix} L = -\frac{1}{2} e^{2i(\alpha+\rho)} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \\ \text{and} \\ M = +\frac{1}{2} e^{2i\alpha} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$1\,c - \begin{pmatrix} \rho = \rho' \pm \pi/2 \\ \gamma = \gamma' = \pi/2 \\ \alpha = \alpha' \\ \delta_1 = +\pi/2 \\ \theta = +\pi/4 \text{ or } -3\,\pi/4 \\ \delta_2 = 0 \end{pmatrix} \text{ and } \begin{pmatrix} \rho = \rho' \pm \pi/2 \\ \gamma = \gamma' = 0 \\ \alpha = \alpha' \\ \delta_1 = -\pi/2 \\ \theta = -\pi/4 \text{ or } 3\,\pi/4 \\ \delta_2 = \pi \end{pmatrix}$$

$$\text{gives} \begin{pmatrix} L = +\frac{1}{2} e^{2i(\alpha+\rho)} \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \\ \text{and} \\ M = -\frac{1}{2} e^{2i\alpha} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$1\,d - \begin{pmatrix} \rho = \rho' \pm \pi/2 \\ \gamma = \gamma' = \pi/2 \\ \alpha = \alpha' \\ \delta_1 = +\pi/2 \\ \theta = +\pi/4 \text{ or } -3\,\pi/4 \\ \delta_2 = \pi \end{pmatrix} \text{ and } \begin{pmatrix} \rho = \rho' \pm \pi/2 \\ \gamma = \gamma' = 0 \\ \alpha = \alpha' \\ \delta_1 = -\pi/2 \\ \theta = -\pi/4 \text{ or } +3\,\pi/4 \\ \delta_2 = 0 \end{pmatrix}$$

$$\text{gives} \begin{pmatrix} L = -\frac{1}{2} e^{2i(\alpha+\rho)} \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \\ \text{and} \\ M = -\frac{1}{2} e^{2i\alpha} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$2\,a - \begin{pmatrix} \rho = \rho' \\ \gamma = \gamma' = 0 \\ \alpha = \alpha' + \pi/2 \\ \delta_1 = 0 \\ \theta = +\pi/4 \text{ or } -3\,\pi/4 \end{pmatrix}$$

$$\text{gives} \begin{pmatrix} L = +\frac{1}{2} e^{2i\alpha'} \begin{pmatrix} 1 - \cos\delta_2 e^{2i\rho} & -(1 + \cos\delta_2 e^{2i\rho}) \\ -(1 + \cos\delta_2 e^{2i\rho}) & 1 - \cos\delta_2 e^{2i\rho} \end{pmatrix} \\ \text{and} \\ M = -\frac{1}{2} i \sin\delta_2 e^{2i(\alpha'+\rho)} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$2\,b - \begin{pmatrix} \rho = \rho' \\ \gamma = \gamma' = 0 \\ \alpha = \alpha' + \pi/2 \\ \delta_1 = \pi \\ \theta = +\pi/4 \text{ or } -3\,\pi/4 \end{pmatrix}$$

$$\text{gives} \begin{pmatrix} L = +\frac{1}{2} e^{2i\alpha} \begin{pmatrix} -(1+\cos\delta_2 e^{2i\rho}) & -(-1+\cos\delta_2 e^{2i\rho}) \\ -(-1+\cos\delta_2 e^{2i\rho}) & -(1+\cos\delta_2 e^{2i\rho}) \end{pmatrix} \\ \text{and} \\ M = -\frac{1}{2} i \sin\delta_2 e^{2i(\alpha'+\rho)} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$2\,c - \begin{pmatrix} \rho = \rho' \\ \gamma = \gamma' = 0 \\ \alpha = \alpha' + \pi/2 \\ \delta_2 = 0 \\ \theta = -\pi/4 \text{ or } +3\,\pi/4 \end{pmatrix} \text{ gives } \begin{pmatrix} L = +\frac{1}{2} e^{2i\alpha} \begin{pmatrix} \cos\delta_1 - e^{2i\rho} & \cos\delta_1 + e^{2i\rho} \\ \cos\delta_1 + e^{2i\rho} & \cos\delta_1 - e^{2i\rho} \end{pmatrix} \\ \text{and} \\ M = +\frac{1}{2} i \sin\delta_1 e^{2i\alpha} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$2\,d - \begin{pmatrix} \rho = \rho' \\ \gamma = \gamma' = 0 \\ \alpha = \alpha' + \pi/2 \\ \delta_2 = \pi \\ \theta = -\pi/4 \text{ or } +3\,\pi/4 \end{pmatrix} \text{ gives } \begin{pmatrix} L = +\frac{1}{2} e^{2i\alpha} \begin{pmatrix} \cos\delta_1 + e^{2i\rho} & \cos\delta_1 - e^{2i\rho} \\ \cos\delta_1 - e^{2i\rho} & \cos\delta_1 + e^{2i\rho} \end{pmatrix} \\ \text{and} \\ M = +\frac{1}{2} i \sin\delta_1 e^{2i\alpha} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$2\,e - \begin{pmatrix} \rho = \rho' \\ \gamma = \gamma' = \pi/2 \\ \alpha = \alpha' + \pi/2 \\ \delta_1 = 0 \\ \theta = -\pi/4 \text{ or } +3\,\pi/4 \end{pmatrix}$$

$$\text{gives} \begin{pmatrix} L = -\frac{1}{2} e^{2i\alpha} \begin{pmatrix} -(1-\cos\delta_2 e^{2i\rho}) & 1+\cos\delta_2 e^{2i\rho} \\ 1+\cos\delta_2 e^{2i\rho} & -(1-\cos\delta_2 e^{2i\rho}) \end{pmatrix} \\ \text{and} \\ M = +\frac{1}{2} i \sin\delta_2 e^{2i(\alpha'+\rho)} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$2\,f - \begin{pmatrix} \rho = \rho' \\ \gamma = \gamma' = \pi/2 \\ \alpha = \alpha' + \pi/2 \\ \delta_1 = \pi \\ \theta = -\pi/4 \text{ or } +3\,\pi/4 \end{pmatrix}$$

$$\text{gives} \begin{pmatrix} R = +\frac{1}{2} e^{2i\alpha} \begin{pmatrix} -1+\cos\delta_2 e^{2i\rho} & -(1-\cos\delta_2 e^{2i\rho}) \\ -(1-\cos\delta_2 e^{2i\rho}) & -1+\cos\delta_2 e^{2i\rho} \end{pmatrix} \\ \text{and} \\ T = +\frac{1}{2} i \sin\delta_2 e^{2i(\alpha'+\rho)} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$2\,g - \begin{pmatrix} \rho = \rho' \\ \gamma = \gamma' = \pi/2 \\ \alpha = \alpha' + \pi/2 \\ \delta_2 = 0 \\ \theta = +\pi/4 \text{ or } -3\pi/4 \end{pmatrix} \quad \text{gives} \quad \begin{pmatrix} L = -\frac{1}{2} e^{2i\alpha'} \begin{pmatrix} -\cos\delta_1 + e^{2i\rho} & -(\cos\delta_1 + e^{2i\rho}) \\ -(\cos\delta_1 + e^{2i\rho}) & -\cos\delta_1 + e^{2i\rho} \end{pmatrix} \\ \text{and} \\ M = -\frac{1}{2} i \sin\delta_1 e^{2i\alpha'} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

$$2\,h - \begin{pmatrix} \rho = \rho' \\ \gamma = \gamma' = \pi/2 \\ \alpha = \alpha' + \pi/2 \\ \delta_2 = \pi \\ \theta = +\pi/4 \text{ or } -3\pi/4 \end{pmatrix} \quad \text{gives} \quad \begin{pmatrix} L = \frac{1}{2} e^{2i\alpha} \begin{pmatrix} -(\cos\delta_1 + e^{2i\rho}) & -\cos\delta_1 + e^{2i\rho} \\ -\cos\delta_1 + e^{2i\rho} & -(\cos\delta_1 + e^{2i\rho}) \end{pmatrix} \\ \text{and} \\ M = -\frac{1}{2} i \sin\delta_1 e^{2i\alpha'} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \end{pmatrix}$$

Changing the condition on α by $\alpha = \alpha' - \pi/2$ gives eight other solutions 2′ a ... 2′ h obtained from the previous ones by changing the sign of M. The solution used in this work corresponds to solution 2′ e when setting ρ to 0.

Eight other solutions exist in branch 2, where $\delta_1 = 0$ or π, $\delta_2 = 0$ or π and θ is a free parameter, but give $M = 0$, meaning that the two directions ignore each other completely : in this case, the 2D system degenerates into two independent classes of 1D systems along the two orthogonal directions.

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