Growth, self-randomization, and propagation in a Lorentz lattice gas

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A systematic study is carried out of a Lorentz lattice gas in order to model the growth dynamics of order-disorder interfaces. In the model, a particle, initially at the origin, moves on the bonds of an initially ordered square lattice, with sites covered by periodically repeated square blocks of 1, 4, or 9 right or left scattering rotators, whose orientations change after collisions with the particle. Depending then on the initial conditions of the blocks and the particle, one observes the following: (a) the particle randomizes the rotator orientations completely, in an ever growing disordered "liquid" phase inside the ordered "solid" phase on the rest of the lattice; (b) the particle propagates suddenly after a transient randomization period as in (a); or (c) the particle propagates through the ordered lattice immediately. A simple picture for the growth of the randomized region, which proceeds via an interface of fractal dimension 0.75, is discussed. The nature of the propagation for the cases mentioned can be modified by collisions with impurities.

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The static and dynamical properties of an interface between ordered and disordered phases, e.g., solid and liquid, have been studied by a wide variety of stochastic models, where random noise in the interface growth process is introduced to generate the rough and irregular properties that the interface of a real physical system is known to possess. Even though the microscopic dynamical equations for particle motions are ultimately deterministic, it seems inevitable to introduce a probabilistic element, given the complicated nature of the interface dynamics. In this paper, however, we propose a *deterministic* Lorentz lattice gas model to study the growth of the order-disorder, or solid-liquid, interface. In particular, we study how, by the motion of a single moving particle, a drop of liquid inside an infinite solid grows and gradually melts the solid. It turns out that much of the desired irregular nature is spontaneously generated by this simple deterministic model. We also found that the outcome will depend on the structure of the basic block that forms the periodic solid phase by translations. For certain blocks, a steady growth of the liquid region is observed for the entire duration of our calculations. This represents a model for interface growth. For others, an abrupt onset of a wavelike propagation through the lattice is found after a transient time. While we do not have an immediate physical correspondence of the propagating mode, we believe this is a combined consequence of the periodicity of the lattice and the collective motion of the particle and the flipping rotator medium in which it moves. Thus it could have potential applications to physical systems that happen to satisfy these two conditions.

In the usual Lorentz lattice gas, one considers the motion of one particle in discrete time steps from site to site on a lattice, *randomly* occupied by scatterers, which scatter the particle, upon collision, according to certain scattering rules. In a number of previous publications, Lorentz lattice gases have been considered on a variety of lattices for a number of deterministic scattering rules. New types of diffusion, not found in a continuum system, were discovered [1]. In this paper, we consider the motion of one particle on a square lattice *regularly* occupied by scatterers: flipping rotators (FR's). Here the particle will scatter to its right (left) upon collision with a right (left) rotator, which flips, i.e., changes orientation, after the collision from a right (left) to a left (right) rotator, respectively.

While in the case of a lattice randomly occupied by scatterers an average can be carried out over all possible random configurations consistent with a given number of right and left scatterers, for a lattice regularly occupied by scatterers, no such average occurs. Nevertheless, we will see that certain random properties of the lattice gas, i.e., a liquid, will result from the deterministic motion of the particle on the lattice initially ordered. To be precise, we will consider here, in particular, the case of a particle moving from the origin on an infinite square lattice fully covered by square blocks of right (R) and left (L) scatterers of increasing size of n lattice units. In other words, the types of scatterers on the lattice are obtained by translating the $n\times n$ basic block of scatterers to cover the whole lattice. Thus the lattice is invariant under vertical or horizontal translations of n lattice units.

Although our main interests here are the ever growing liquid regions, we will, for systematic reasons, discuss the behavior of the Lorentz lattice gas as a function of increasing block size. As indicated before, for certain basic blocks, the particle could settle into a propagation mode.

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Once in this mode, the rotator configuration in a restricted neighborhood around the current position of the particle will repeat itself indefinitely after displacement of the particle in a fixed direction in a fixed number of time steps, which we call a period. This self-repetition provides the mechanism by which the particle propagates indefinitely on the lattice in a certain direction. The propagation is characterized by the displacement vector of the particle during one period: the propagation distance is the length of the displacement vector, the propagation direction is given by that of the displacement vector, and the propagation velocity is the ratio of the propagation distance and the period.

Our model is discrete in both space and time and the discrete space step from one lattice site to the next, as well as the discrete time step, provide the units for distances and times, respectively. Thus no explicit labeling of units is necessary for all the quantities and figures in the following.

(1) The case of a lattice occupied by a R or L FR of period 1, i.e., a lattice fully occupied by either R or L FR's [cf. Fig. 1(a)] has been discussed before [1(c)]. This model is identical to that of an ant walking on a square lattice considered earlier by Langton [2]. In this case one finds that, after a transient motion of 9977 time steps, the particle settles in a periodic propagation mode of period 104, a width of 5 lattice sites, and a propagation distance of $2\sqrt{2}$. This is case (b) mentioned in the Abstract. During the propagation the particle moves forward and backward, repeating 43 lattice sites per period. Here repetition is defined as the smallest number of common sites visited by the particle in one period, which were also visited in (a) previous period(s), for all choices of the starting point of the period. The propagation is similar to but more complicated than that discussed before on a triangular lattice occupied by FR's [1(a),(b)]. We note that the direction of propagation is always along a diagonal and only depends on the type of scatterer covering the lattice (R or L) and the initial direction of the particle velocity.

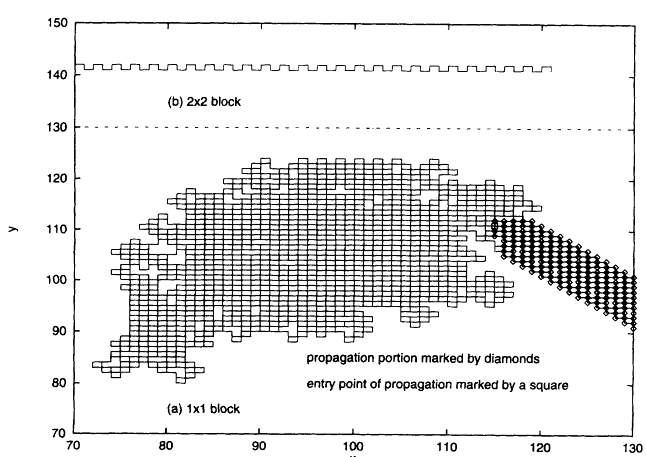

FIG. 1. (a) Propagation on a lattice initially with only L rotators. The particle starts at (100,100) due north and begins to propagate after a transient of 9977 time steps. (b) The immediate propagation (meander) of a particle on a lattice with alternating rows of R and L rotators initially.

(2) In the case of a lattice occupied by (2×2) blocks of period 2, only three cases have to be distinguished, with patterns having only one L, two L's in one row (column), or two L's in a diagonal, respectively. They all lead to immediate propagations, with periods 8, 4, and 2, and propagation velocities $\frac{1}{4}$, $\frac{1}{2}$, and $1/\sqrt{2}$, respectively, either along the horizontal or vertical axes (meander) or a diagonal (zigzag), depending on the arrangements of the scatterers and the initial phase, i.e., initial position and velocity of the particle [cf. Fig. 1(b)]. This corresponds to case (c) mentioned in the Abstract.

(3) In the case of a lattice occupied by (3×3) blocks of period 3, there are 2^9 different scatterer arrangements, nine initial particle positions with four different particle velocities each. By symmetry, only 13 scatterer arrangements have to be considered for 36 initial particle phases. A given scatterer arrangement leads to the same asymptotic motion of the particle up to a rotation or translation, independent of the initial phase of the particle. However, the way this motion is reached, i.e., the particle's transient behavior, depends strongly on the particle's initial phase. The results are summarized in Table I.

For ten FR configurations, propagation occurs before 10^9 time steps, the maximum time we considered, while for three FR configurations no propagation was found up to that time. We first discuss these three nonpropagating cases, which constitute case (a) mentioned in the Abstract.

(A) The basic result of the motion of the particle from the origin over the lattice in the course of time can then be described as the progressing conversion of a regularly occupied lattice to a randomly occupied lattice. Alternatively, one can consider it as the gradual melting from the inside of an ordered "solid" into a steadily growing "liquid" region, a description we will use here for convenience (cf. Fig. 2). In fact, if we define at time t the area $A(t)$ of the liquid region as the number of distinct sites visited by the particle and the boundary $B(t)$ of the liquid region as the number of the sites inside the liquid region which have at least one (solid) neighbor which has not been visited, then for roughly $t>5000$ one finds the power laws

$$A(t)\sim t^{\alpha} \quad \text{with } \alpha=0.75\ , \tag{1a}$$

$$B(t)\sim t^{\beta} \quad \text{with } \beta=0.50\ , \tag{1b}$$

where α and β have been determined by least squares fits. The fact that $B\sim A^{\beta/\alpha}$ with $\beta/\alpha\simeq\frac{2}{3}\neq\frac{1}{2}$ suggests that the boundary is a fractal with dimension $2\beta/\alpha\simeq\frac{4}{3}$. This is confirmed by direct measurement. For t larger than roughly 5000, the liquid region is essentially a simply connected region, with only a few nonvisited sites mainly near the boundary.

That the rotator distribution inside the liquid region is indeed random can be established by considering the two point rotator orientation autocorrelation function

$$F(\mathbf{r},t)=\sum_{\mathbf{r}_1,\mathbf{r}_2}{}' f(\mathbf{r}_1,t)f(\mathbf{r}_2,t)\Big/\sum_{\mathbf{r}_1,\mathbf{r}_2}{}' 1\ .$$

TABLE I. Top row lists the positions of L's in 3×3 blocks, by numbering the sites in a block from 1 to 9 and from left to right, respectively, so that the sites in the first row are labeled 1,2,3, those in the second row 4,5,6, and those in the third row 7,8,9. We characterize each block by the position(s) of the left rotators, the others all being right rotators. The nonpropagating patterns are indicated by ∞.

Positions of L rotators	None	1	1,2	1,9	1,2,3	1,2,5	1,2,9	1,5,9	1,2,3,4	1,2,4,5	1,2,5,9	1,3,4,9	1,4,8,9
Period	104	164	∞	598	4	68	14	2	4	∞	2	414	∞
Repetition	43	4	∞	1	0	1	1	0	0	∞	0	54	∞
Average transient	9977	3677	∞	128	0	54	62	0	0	∞	0	40 049	∞
Velocity	$\frac{\sqrt{2}}{52}$	$\frac{3\sqrt{2}}{299}$		$\frac{3\sqrt{34}}{598}$	$\frac{1}{2}$	$\frac{3\sqrt{2}}{34}$	$\frac{3\sqrt{2}}{14}$	$\frac{\sqrt{2}}{2}$	$\frac{1}{2}$		$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{10}}{138}$	

Here $f(\mathbf{r},t)=+1$ or -1, if there is a R or L rotator, respectively, on the site $\mathbf{r}$ at time t, and the prime on the summation sign indicates that the summation is carried out over $\mathbf{r}_1$ and $\mathbf{r}_2$ in the entire liquid region with the restriction that $\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1$. Figure 3 shows a typical $F(\mathbf{r},t)$ for $\mathbf{r}=(1,0)$ which vanishes after about 5000 time steps. Also plotted is $t/A(t)$, the number of collisions per lattice site, showing that at $t=5000$ each scatterer has been visited about five times, which suffices to randomize them. Similar results obtain for three and four point correlation functions.

Not only the scatterer configuration in the liquid region is random after $t\simeq5000$; the particle trajectory is also. One way of seeing this is by cutting the trajectory at time T into n large sections of τ time steps, so that $T=n\tau$. We consider then the distribution $P(\mathbf{r},\tau)$ of displacements $\mathbf{r}_{n\tau}-\mathbf{r}_{(n-1)\tau}$ in those sections for $n=1,2,\ldots,T/\tau$. Using that $P(\mathbf{r},\tau)$ in the liquid region does not depend on the direction of $\mathbf{r}$, we define a radial distribution function $\hat{P}(r,\tau)=2\pi rP(\mathbf{r},\tau)$ for τ larger than roughly 1000; $\hat{P}$ corresponds to that of a Gaussian distribution with a diffusion coefficient $D_{\mathrm{RL}}\approx0.35$ (cf. Fig. 4), where RL refers to random liquid. This value of D is larger than that for the corresponding random walk (RW), $D_{\mathrm{RW}}=0.25$, but equal to that found before [1(a)] for the diffusion of a particle in a *random* distribution of an equal number of R and L flipping rotators on a fully occupied square lattice. That $D_{\mathrm{RL}}>D_{\mathrm{RW}}$ can be understood on the basis of the impossibility of the occurrence of certain sequences of collisions in the FR model which are permitted in the RW, e.g., the impossibility of five successive R (or L) turns, leading to an effective "short-range repulsive correlation" between sites visited by the particle. The same results for $\hat{P}(r,\tau)$ are obtained for the displacements of particles randomly put on the RL.

Another way of establishing the randomness of the particle trajectory is to consider correlations instead of displacements. Defining $h_i=+1$ or -1 if the particle

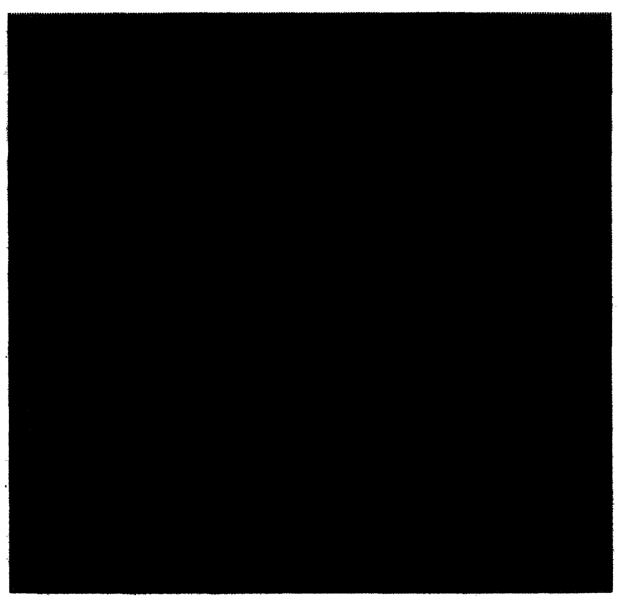

FIG. 2. Liquid (inner region) and solid (outer region) for a typical nonpropagating pattern [(1,2,4,5) in Table I] at $t=4\,660\,000$. The square shown is a 720×720 part of the lattice. The rotator distribution inside the liquid is random with no spatial correlations. The boundary between the liquid and solid is a fractal with dimension 1.33. Black is R, white is L.

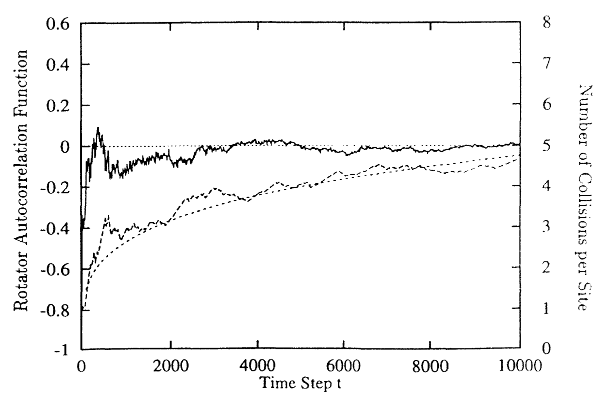

FIG. 3. The correlation function $F(\mathbf{r},t)$ (solid line) with $\mathbf{r}=(1,0)$ as a function of t for nearest neighbor scatterers at distance 1 inside the growing liquid region. It reaches equilibrium (zero) and fluctuates around it after about 5000 time steps, indicating that the liquid is then truly random. The number of collisions per site, i.e., $t/A(t)$ (dashed line), shows that the liquid is randomized after about five collisions per site; its $t^{1/4}$ asymptotic behavior is also plotted [cf. Eq. (1a)].

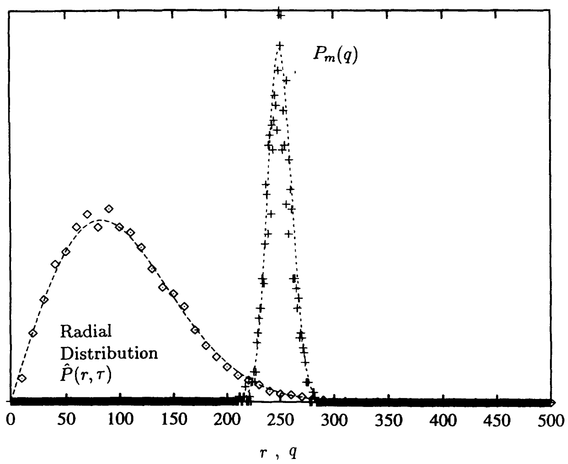

FIG. 4. Radial probability distribution $\hat{P}(r,\tau)$ for the distance r the particle travels in an interval τ of 10 000 time steps (diamonds). Total time T considered is around 100 million time steps. The dashed line corresponds to a Gaussian distribution with diffusion coefficient $D_{\text{RL}}=0.35$. Also shown is the probability distribution $P_m(q)$ (crosses) to have q +1's and $(m-q)$ −1's in an interval of m binary numbers generated from a typical particle trajectory. Here $m=500$ and $P_m(q)$ is determined from 2000 such intervals. The dotted line is the binomial distribution for an ideal random number generator. Note that r and q are plotted on the same horizontal axis. The points were determined from a single trajectory. The agreement between points and curve can be improved by choosing larger trajectories.

TABLE II. Comparison of the properties of the particle trajectories of a random walk (RW) and a walk in a liquid of randomly distributed rotators (RL). τ_{esc} is the mean escape time of a particle, starting at the origin, from a circle of radius R centered at the origin. Values of R between 100 and 1000 lattice distances have been used. The average is taken over typically 5000 random distributions of rotators inside the circle. $t/A\,\log_{10}t$ is the inverse of the proportionality constant in the relation number of visited sites $A \sim t/\ln t$ (for a RW see [4]). $\Delta(t)$ is the mean square displacement. The probability distribution of the displacements is Gaussian in both cases.

Walk	τ_{esc}	$t/A\ln t$	$\Delta(t)$	D	$\hat{P}(r,t)$
RW	R^2	2.80	$4Dt$	0.25	Gaussian
RL	$0.75R^2$	3.15	$4Dt$	0.35	Gaussian

makes a R or a L turn, respectively, at time i, we consider the particle turn autocorrelation function $G(j)=\sum_{i=1}^{T} h_i h_{i+j}/T$ for all j and $T\rightarrow\infty$; T is about 10^8 in practice. $G(j)$ is plotted in Fig. 5. While there are correlations for $j<40$ due to memory effects, these become negligible for $j\geq 40$, where $G(j)$ becomes indistinguishable from an ideal random number generator. In fact, Fig. 5 suggests that the randomness of the binary number sequence $h_i, h_{i+40}, h_{i+80}, \ldots$ can be tested by dividing it into adjacent intervals of m numbers each and looking for the probability $P_m(q)$ to find q +1's and

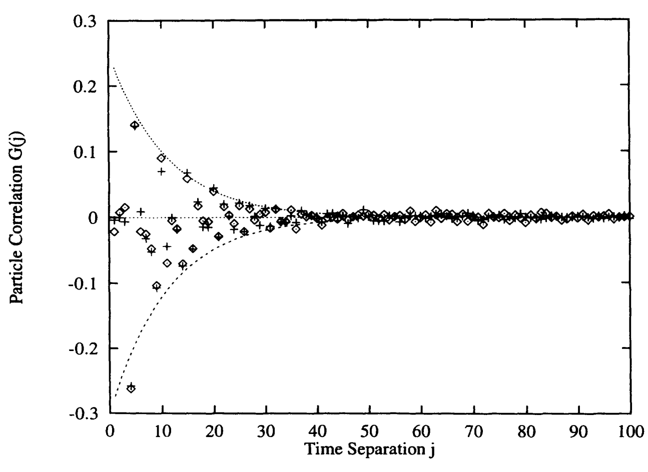

FIG. 5. Particle turn autocorrelation function $G(j)$. The strong correlations for $j<40$ show the significant difference between a walk in a random distribution of our rotators and a true random walk. The upper and lower envelopes of the correlation function appear to approach zero exponentially, and can be fitted by $0.25\exp(-j/11)$ and $-0.30\exp(-j/11)$, respectively. The results from two basic 3×3 block patterns [(1,2) (diamonds) and (1,2,4,5) (pluses) of Table I] are shown. They are indistinguishable within statistical errors.

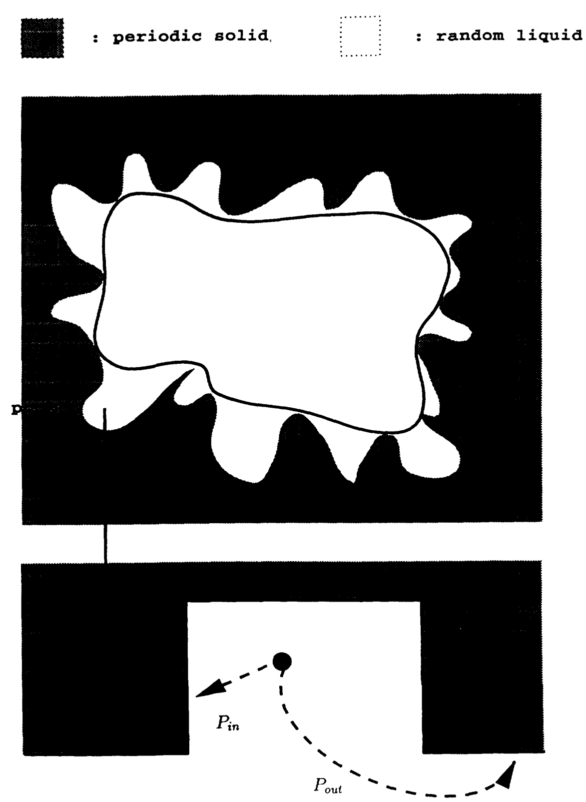

FIG. 6. Pockets are idealized by rectangles with width w and height h. The particle will escape from the pocket or collide with its wall with probabilities P_{out} and P_{in}, respectively.

$(m-q)$ -1's in these intervals, which is shown in Fig. 4. We find that $P_m(q)$ approaches $\binom{m}{q}$, the binomial distribution, as should be. Thus after about 5000 steps a self-randomization of the particle-scatterer system has taken place, since the particle then moves randomly in a random medium of its own creation on the otherwise still ordered lattice. The motion of the particle in the RL is in the same universality class as a RW, but with different amplitude (cf. Table II).

We conclude our discussion of the RL by providing a simple growth mechanism consistent with the power laws Eqs. 1(a) and 1(b). We first remark that the basic growth process suggested by the computer simulations is the following: upon reaching the liquid boundary, the particle will grow a small liquid pocket into the solid region, after which the particle reenters the bulk liquid to grow another such pocket on its next encounter with the boundary, etc. We denote the average pocket area a and the average collision rate with the liquid boundary $1/\tau(R)$, where $R\sim\sqrt{A}$ defines the size of the liquid region. We remark that, in terms of R, Eq. (1b) becomes $B(R)\sim R^{\alpha'}$ with $\alpha'=2\beta/\alpha\simeq 1.33$, so that the liquid boundary is a fractal, while the liquid area $A(R)\sim R^2$ is not. To obtain $\tau(R)$ we construct a smooth line through the boundary and idealize the resulting pockets formed by the real boundary around this line by rectangles of average height h and width w, as illustrated in Fig. 6. Then the length of the boundary $B(R)\sim hR/w\sim R^{\alpha'}$, so that $h/w\sim R^{\alpha'-1}$. Next we note that a particle inside a pocket can either escape into the bulk liquid with probability P_{out} and average liquid boundary recollision time τ_{out}, or hit a wall of the pocket, with corresponding P_{in} and τ_{in}, respectively (cf. Fig. 6). Then

$$\tau(R)=\tau_{\text{in}}(R)P_{\text{in}}(R)+\tau_{\text{out}}(R)P_{\text{out}}(R)\ .$$

Since for sufficiently large R, $\tau_{\text{out}}P_{\text{out}}\gg\tau_{\text{in}}P_{\text{in}}$, because P_{out} and $\tau_{\text{in}}P_{\text{in}}$ stay finite for $R\to\infty,\tau(R)\approx\tau_{\text{out}}(R)P_{\text{out}}(R)$. One would expect that for such R, $\tau_{\text{out}}(R)\sim R^2(1/R)$ and $P_{\text{out}}(R)\sim w/h$, which is confirmed numerically. This leads to

$$\tau(R)\sim Rw/h\sim RR^{1-\alpha'}=R^{2-\alpha'}\ .$$

Thus

$$dA(R)/dt\sim R\,dR/dt\simeq R^{\alpha'-2}\ ,$$

leading to $R\sim t^{1/(4-\alpha')}$ and finally $B(t)\sim t^{\alpha'/(4-\alpha')}$ and $A(t)\sim t^{2/(4-\alpha')}$, which gives Eq. (1) for $\alpha'=\frac{4}{3}$. There is therefore only one independent exponent, because of the scaling relation $\alpha=2/(4-\alpha')$, or equivalently $2\alpha-\beta=1$.

(B) We now turn to the ten propagating cases summarized in Table I. The duration of the transients before

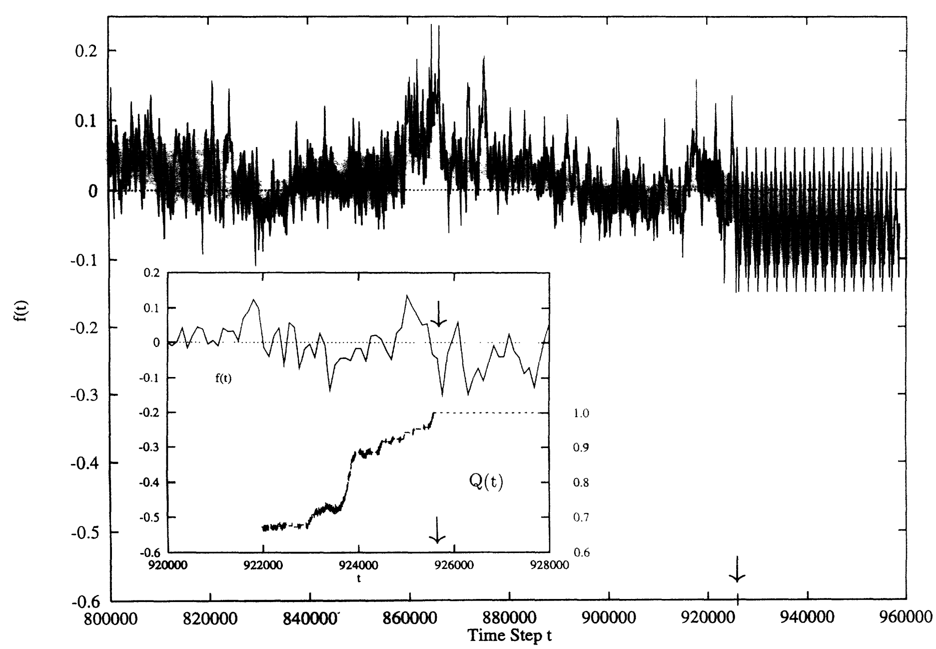

FIG. 7. Nearest-neighbor rotator orientation correlation function $f(t)$ averaged over all visited sites in a box of 50×50 sites and moving with the particle as a function of time. The transition happens at $t_p=925\,589$. The propagation period is 1926 steps. Shown in the inset is a quantity $Q(t)$ on an extended time scale and defined as follows. For propagation to start at t_p, a certain (critical) rotator configuration in a neighborhood around the particle is necessary. This holds in particular at the transition time t_p. In order to see how this critical neighborhood is reached in time, we define $Q(t)$ as the fraction of all those sites in the critical neighborhood at time $t<t_p$ which are occupied by the same type of rotator as the critical one has at t_p, and plot it as a function of t. By definition, $Q(t_p)=1$. For comparison, we plot $f(t)$ with it on the same extended time scale. The arrows indicate the position of t_p.

propagation strongly depends on the initial phase of the particle. In Table I, the average transient times for all 36 different initial particle phases for a given scatterer configuration are given. For blocks smaller than (4×4), the propagating mode is independent of the initial particle phase, however. We note that, if propagation occurs after more than 5000 time steps, the transient regime will be a random liquid as described above. Second, we remark that the transition to propagation occurs suddenly at a time t_p. That is, we have not been able to find any indication of an approach to this transition: it seems that the particle starts propagating from one instant of time to the next without any warning signal. To illustrate the sudden transition at t_p from random to periodic propagating behavior, we define a function $f(t)$, where f could be, for example, the x or y coordinate of the particle, or the R (L) turn the particle makes at time t, or a more complicated property, such as that shown in Fig. 7. We note that in Fig. 7 $f(t)$ appears to be equally irregular right up to t_p, after which the function suddenly becomes periodic and exhibits regular patterns. Thus one could say that it appears that the phase point representing the particle-scatterer system moves in the phase space of the system, unaware of the presence of (a) hole(s) in which it can fall—which indicates that the particle starts propagating—until actually falls into one.

We conclude with a number of open questions.

(1) In view of the above, we have not been able so far to give a mechanism that leads to propagation. In particular, we do not know for which initial conditions of lattice and particle liquid growth or propagation will occur on a lattice periodically occupied by scatterers.

(2) The propagating modes found here from a given initial particle state are not the only ones that can occur on a given regularly occupied lattice. Intercepting, for instance, the propagation on a lattice regularly covered by a 3×3 block, by inserting a 35×10 block of R rotators, leads after a transient period to a different propagating mode in a different direction than before (cf. Fig. 8). We do not know how many of such "excited" propagating modes exist for a given regularly covered lattice. For a (1×1) block only one propagating mode appears to occur [1(b),2].

(3) In addition to the systematic study of the blocks discussed above, we have studied a number of (4×4), (5×5), and (6×6) blocks. In general, the behavior is then similar to that of the smaller blocks, except that different propagating modes can occur *ab initio* by simply changing the initial state of the particle.

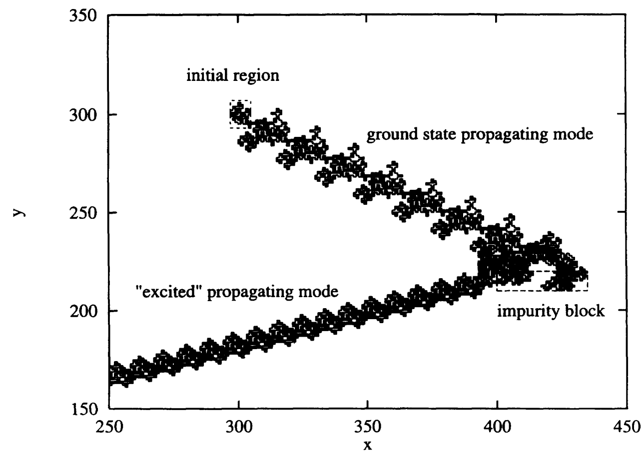

FIG. 8. Trajectory of a particle [pattern (1,9) in Table I, with initial particle position 1 and velocity due east] starting from lattice site (300,300) in the "ground state" propagating mode, after a transient of 151 time steps. After seven periods, it is then intercepted by a block of impurities of 35×10 R rotators with the lower left corner located at (400,210). An "excited state" propagating mode with a different period (312) emerges after the interception. Not all the sites in the impurity region are visited.

(4) The motion of two particles simultaneously on a periodically ordered lattice will depend on the initial phases of the particles and can lead not only to liquid regions, but also, if propagation occurs, to a scattering of the two particles off each other, or to new joint collective motions [3]. In fact, two propagating particles can form, upon collision, a joint periodic orbit. A third particle, intersecting this orbit, can effect a "dissociation" and lead to three propagating particles again. Clearly, the results reported here seem to indicate a very rich and complex behavior of what appears to be a rather simple system.

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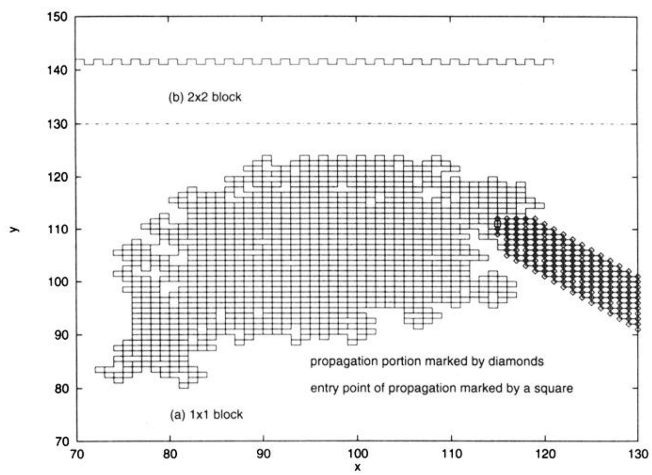

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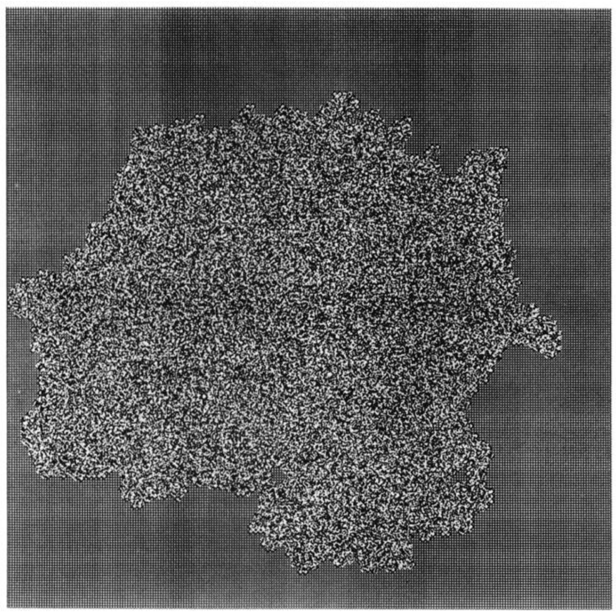

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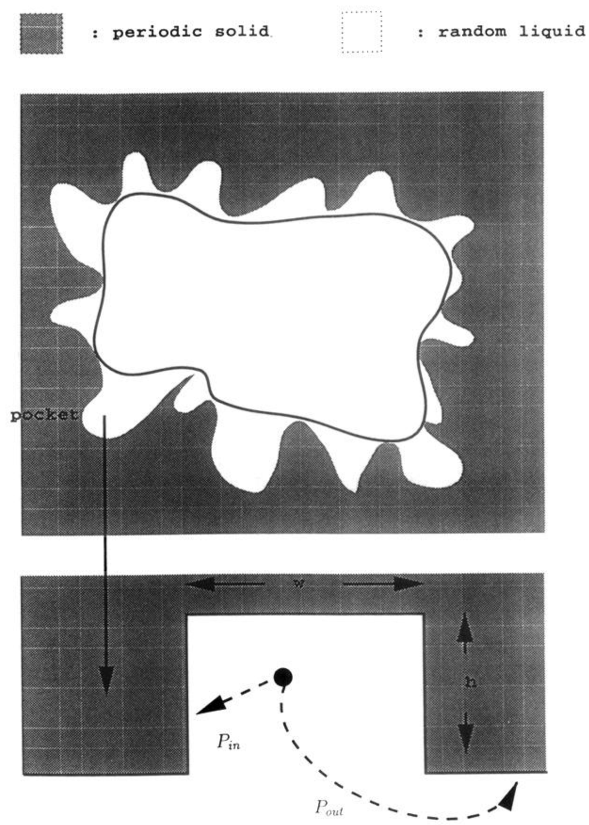

FIG. 6. Pockets are idealized by rectangles with width w and height h. The particle will escape from the pocket or collide with its wall with probabilities P_{out} and P_{in}, respectively.

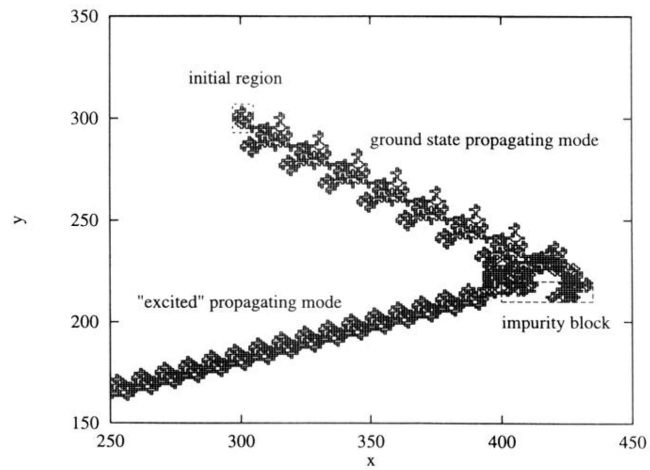

FIG. 8. Trajectory of a particle [pattern (1,9) in Table I, with initial particle position 1 and velocity due east] starting from lattice site (300,300) in the "ground state" propagating mode, after a transient of 151 time steps. After seven periods, it is then intercepted by a block of impurities of 35×10 R rotators with the lower left corner located at (400,210). An "excited state" propagating mode with a different period (312) emerges after the interception. Not all the sites in the impurity region are visited.