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## Multiphase partitions of lattice random walks

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Abstract – Considering the dynamics of non-interacting particles randomly moving on a lattice, the occurrence of a discontinuous transition in the values of the lattice parameters (lattice spacing and hopping times) determines the uprisal of two lattice phases. In this letter we show that the hyperbolic hydrodynamic model obtained by enforcing the boundedness of lattice velocities derived in GIONA M., *Phys. Scr.*, **93** (2018) 095201 correctly describes the dynamics of the system and permits to derive easily the boundary condition at the interface, which, contrarily to the common belief, involves the lattice velocities in the two phases and not the phase diffusivities. The dispersion properties of independent particles moving on an infinite lattice composed by the periodic repetition of a multiphase unit cell are investigated. It is shown that the hyperbolic transport theory correctly predicts the effective diffusion coefficient over all the range of parameter values, while the corresponding continuous parabolic models deriving from Langevin equations for particle motion fail. The failure of parabolic transport models is shown via a simple numerical experiment.

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Lattice models of particle dynamics represent a robust conceptual backbone in statistical theory of non-equilibrium processes, finding broad and diversified applications in all the branches of physics [1,2]. They constitute a simple gedanke experimental environment in order to derive, from simple local interaction rules, the corresponding hydrodynamic models in a continuous spacetime setting [3,4].

Even in the case of systems of non-interacting particles, a rich variety of possible phenomenologies arises, associated with lattice heterogeneities and impurities [5], randomly distributed multisite structures [6,7], disorder, percolation and phase transitions [8], anomalous behavior induced by a continuous distribution of hopping times and hopping lengths (that can be treated within the framework of Continuous Time Random Walk) [9,10], etc.

In recent years, lattice heterogeneity has been studied in connection with infiltration dynamics, and solute partition in two lattice phases, defined by the decomposition of the lattice in two subsets possessing different lattice parameters [11–16]. The latter problem has great current interest in biological applications involving active swimmers moving in non-uniform fields modulating their mobilities [17], and is connected to fundamental problems involving the stochastic modeling of non-equilibrium phenomena, associated with the proper choice of the most suitable stochastic calculus (Ito, Stratonovich, Hänggi-Klimontovich) [18,19], and with the properties of the equilibrium invariant densities and their connection with local transport properties [20].

Although the current research focus is mostly oriented towards particle motion determining the occurrence of anomalous diffusive phenomena [12], the case of the simplest possible model of lattice random walk involving noninteracting particles has shown that some interesting properties are still to be unveiled, especially as regards its continuous hydrodynamic description. By definition, a lattice random walk is parametrized with respect to an operational time n, counting the number of transitions occurring in the particle motion, and corresponding to the physical time  $t_n$ , by  $t_n = n\tau$ ,  $\tau$  being the constant hopping time. Consequently, a lattice trajectory  $\{x_n\}_{n\in\mathbb{N}}$  is the countable sequence of the lattice positions attained by a particle with respect to the operational time. By considering a space-time continuation of the lattice trajectories, performed by linearly interpolating between two subsequent space time points  $(x_n, t_n)$  and  $(x_{n+1}, t_{n+1})$ , it has been shown recently in [21] that the classical lattice random walk of independent particles can be described

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Fig. 1: Schematic representation of a MuPh-LRW.

in a continuous space-time setting by means of a hyperbolic transport model analogous to those arising in the theory of Generalized Poisson-Kac processes [22,23]. The hyperbolic transport model accounts intrinsically for the finite propagation velocity of the process, and provides an accurate quantitative description not only of the long-term properties but also of the initial stages of the dynamics [21]. In the case of a symmetric lattice random walk, defined by the characteristic site distance  $\delta$  and hopping time  $\tau$  between nearest neighboring sites, the hyperbolic continuous model involves the partial probabilities  $\{p_{\pm}(x,t)\}$ , where  $p_{\pm}(x,t) dx$  is the fraction of particles in the spatial interval (x, x + dx) at time t moving towards the right  $(p_{+})$  or to the left  $(p_{-})$ , satisfying the equations

$$\frac{\partial p_{\pm}(x,t)}{\partial t} = \mp b \, \frac{\partial p_{\pm}(x,t)}{\partial x} \mp \lambda \left[ p_{+}(x,t) - p_{-}(x,t) \right], \quad (1)$$

where  $b = \delta/\tau$ , and  $\lambda = 1/\tau$ . The overall probability density of the process is  $p(x,t) = p_+(x,t) + p_-(x,t)$ , and the associated flux is  $J(x,t) = b [p_+(x,t) - p_-(x,t)]$ .

In this letter, we consider the multiphase extension of the symmetric random walk, as depicted in fig. 1. The MultiPhase Lattice Random Walk, henceforth MuPh-LRW for short, is a simple random walk on a lattice  $\mathbb{Z}$ , in which the physical lattice parameters  $(\delta, \tau)$  admit a sudden transition at some lattice point, say  $z_0 \in \mathbb{Z}$  so that  $(\delta_1, \tau_1)$  holds for  $z < z_0$ , and  $(\delta_2, \tau_2)$  for  $z > z_0$ . The lattice point  $z_0$  represents the interfase separating the two lattice phases.

Within each lattice phase, particle motion is a symmetric LRW, corresponding, in the continuous limit, to an emergent purely diffusive behavior defined by the phase diffusivities  $D_h = \delta_h^2/2\tau_h$ , h = 1, 2. It remains to specify the motion at the interfacial point  $z_0$ . Two cases can occur: i) if the interfacial point is "neutral" with respect to phase selection, so that equal probabilities characterize the jump from  $z_0$  to one of its two nearest neighboring sites, the interface is referred to as *ideal*; ii) if the probabilities of moving from the interface towards the sites of one of the two phases are different, the interface exerts a specific and active selection, and it will be referred to as *non-ideal* or *active*. In this letter we focus exclusively on ideal interfaces.

In a discrete space-time description, the MuPh-LRW corresponds to a simple symmetric LRW defined by the dynamics  $z_{n+1} = z_n \pm 1$  Prob. 1/2, where  $n = 0, 1, \ldots$ , is

the operational lattice time. In a physical setting, indicating with  $x_n$  the particle spatial position, corresponding to the lattice coordinate  $z_n$  and  $t_n$  the physical time, MuPh-LRW corresponds to a subordination of the stochastic lattice motion according to phase heterogeneity. More precisely, let  $C^{(1)}$ ,  $C^{(2)}$  and  $C^{(int)}$  be the disjoint sets of lattice sites  $z_n$  belonging to phase "1", phase "2" and to the interface, respectively. The MuPh-LRW dynamics in the presence of ideal interfaces is defined in the physical space-time by the equations

$$x_{n+1} = x_n + \Delta_n, \quad t_{n+1} = t_n + T_n,$$
 (2)

where

$$\Delta_n = \begin{cases} \delta_1, & \text{if } (z_n \in \mathcal{C}^{(1)}) \cup [(z_n \in \mathcal{C}^{(\text{int})}) \cap (z_{n+1} \in \mathcal{C}^{(1)})], \\ \delta_2, & \text{if } (z_n \in \mathcal{C}^{(2)}) \cup [(z_n \in \mathcal{C}^{(\text{int})}) \cap (z_{n+1} \in \mathcal{C}^{(2)})], \end{cases}$$
(3)

and analogously for  $T_n$ ,

л

$$T_{n} = \begin{cases} \tau_{1}, & \text{if } (z_{n} \in \mathcal{C}^{(1)}) \cup [(z_{n} \in \mathcal{C}^{(\text{int})}) \cap (z_{n+1} \in \mathcal{C}^{(1)})], \\ \tau_{2}, & \text{if } (z_{n} \in \mathcal{C}^{(2)}) \cup [(z_{n} \in \mathcal{C}^{(\text{int})}) \cap (z_{n+1} \in \mathcal{C}^{(2)})]. \end{cases}$$
(4)

This simply means that in a unit operational time, the distance travelled by a particle is  $\delta_1$ , and the time elapsed  $\tau_1$ , if the initial site belongs to phase "1" or if it is an interfacial site and the particle moves towards phase "1", and analogously for phase "2". Embedding the lattice in a continuum,  $x \in \mathbb{R}$ , this essentially means that for points x belonging to phase "1" the velocity b(x) is  $\delta_1/\tau_1$  and for points belonging to phase "2" the velocity is  $\delta_2/\tau_2$ .

Two main questions arise: i) the definition of a continuous hydrodynamic model for MuPh-LRW, and ii), strictly connected to i), the assessment of the proper boundary condition at an ideal interface in a continuous setting of the dynamics. These two issues are closely related to each other. As regards the hydrodynamic description, the hyperbolic approach introduced in [21] can be applied to each phase. This corresponds to consider eq. (1) for each phase, with  $p_{\pm}(x,t)$  substituted by the phase partial concentration  $p_{\pm}^{(h)}(x,t)$ , defined for x within each disjoint domain of definition of the phases, and b and  $\lambda$  with  $b_h = \delta_h / \tau_h$ ,  $\lambda_h = 1/\tau_h$ . This follows also from eq. (2) by considering the subordination of the physical time t with respect to the lattice time n for processes possessing finite propagation velocity (Poisson-Kac processes). In the case of ideal interfaces, there is no active effect of the interface on the partition of solute particles in the two phases, and the hyperbolic approach based on eq. (1) implies the continuity of the partial fluxes across an ideal interface located at  $x_0$ (corresponding to the lattice coordinate  $z_0$ ),

$$b_1 p_{\pm}^{(1)}(x,t)|_{x=x_0} = b_2 p_{\pm}^{(2)}(x,t)|_{x=x_0}.$$
 (5)

The detailed derivation of eq. (5) is developed below. This condition can be further justified by enforcing the lattice representation of the dynamics, consistently with the analysis developed in [24]. Equation (5) obviously predicts the continuity of the normal fluxes at the interface,  $J^{(1)}(x_0,t) = J^{(2)}(x_0,t)$ , and the boundary condition for the overall particle density

$$\left. \frac{p^{(2)}(x,t)}{p^{(1)}(x,t)} \right|_{x=x_0} = \frac{b_1}{b_2} = \frac{\delta_1 \tau_2}{\delta_2 \tau_1}.$$
 (6)

Derivation of eq. (5). – The boundary conditions for MuPh-LRW in the presence of ideal interfaces can be derived in several different ways. In a fully lattice description, MuPh-LRW is solely a simple symmetric walk on  $\mathbb{Z}$ parametrized with respect to the lattice time  $n \in \mathbb{N}$ . Its statistical description involves the probabilities  $P_h^n$  of finding the particle at the lattice site h at the lattice time n, fulfilling the Markov dynamics  $P_h^{n+1} = (P_{h-1}^n + P_{h+1}^n)/2$ . In a spatially continuous representation of the process, where the particle position is defined over the real line, *i.e.*,  $x \in \mathbb{R}$ , the spatial heterogeneity, associated with the different values of  $\delta_h$  in the two lattice phases plays a role. Let  $\Omega_1, \Omega_2$  be the subset of  $\mathbb{R}$ , occupied by phase "1" and phase "2", respectively.  $\Omega_1$  consists of the the union of the intervals  $(z_h, z_{h+1}), z_h \in \mathbb{Z}$ , where either  $z_h$  or  $z_{h+1}$  belong to to  $\mathcal{C}^{(1)}$ , since if, say  $z_h \in \mathcal{C}^{(1)}$ , then by definition of the multiphase lattice structure,  $z_{h+1}$  belongs either to  $\mathcal{C}^{(1)}$  or to  $\mathcal{C}^{(\inf)}$ , and analogously for  $\Omega_2$ . Introduce over the real line the phase function  $\sigma(x)$ , such that  $\sigma(x) = 1$  if  $x \in \Omega_1$ , and  $\sigma(x) = 2$  if  $x \in \Omega_2$ , and let p(x, n) the probability density function continuously parametrized with respect to the spatial coordinate x.

The probability  $P_h^n$  corresponds to the integral of the continuous p(x, n) over an interval centered at  $x_h$  of width  $\delta_{\sigma(x_h)}$ , where  $\sigma(x_h) = 1, 2$ , depending whether the  $x_h$  belongs to phase "1" or "2". Consequently,

$$P_h^n \simeq p(x_h, n) \delta_{\sigma(x_h)}.$$
 (7)

The hyperbolic stochastic model associated with p(x, n), taking a continuation of n towards real values, stems from a local stochastic dynamics given by

$$dx(n) = \delta(x(n))(-1)^{\chi(n,1)}dn \tag{8}$$

where we have set  $\delta(x) = \delta_{\sigma(x)}$ . Equation (8) is the evolution equation for a Poisson-Kac process [25], where  $\chi(n, 1)$ is a Poisson process depending on the real continued time variable n, and characterized by a transition rate equal to 1, the statistical description of which involves the partial probability density functions  $p_{\pm}^{(h)}(x, n)$  in the two lattice phases, h = 1, 2.

The hyperbolic hydrodynamic model expressed with respect to the continuation of the lattice time n towards real values is given by

$$\frac{\partial p_{\pm}^{(h)}(x,n)}{\partial n} = \mp \delta_h \frac{\partial p_{\pm}^{(h)}(x,n)}{\partial x} \mp [p_{+}^{(h)}(x,n) - p_{-}^{(h)}(x,n)],$$
(9)

where each  $p_{\pm}^{(h)}(x,n)$  is defined in the disjoint subsets  $\Omega_h$ , h = 1, 2, Next, account for the time subordination of t with respect to n

$$dt = \tau(x)dn, \tag{10}$$

where

$$\tau(x) = \begin{cases} \tau_1, & x \in \Omega_1, \\ \tau_2, & x \in \Omega_2, \end{cases}$$
(11)

which, in the present case of hyperbolic stochastic dynamics, means

$$\frac{\partial}{\partial n} = \frac{\mathrm{d}t}{\mathrm{d}n} \frac{\partial}{\partial t}.$$
(12)

Consequently, with respect to the physical time t, the balance equations (9) become

$$\frac{\partial p_{\pm}^{(1)}(x,t)}{\partial t} = \mp b_1 \frac{\partial p_{\pm}^{(1)}(x,t)}{\partial t} \mp \lambda_1 \left[ p_{+}^{(1)}(x,t) - p_{-}^{(1)}(x,t) \right],\\ \frac{\partial p_{\pm}^{(2)}(x,t)}{\partial t} = \mp b_2 \frac{\partial p_{\pm}^{(2)}(x,t)}{\partial t} \mp \lambda_2 \left[ p_{+}^{(2)}(x,t) - p_{-}^{(2)}(x,t) \right],$$
(13)

where  $b_h = \delta_h / \tau_h$ ,  $\lambda_h = 1 / \tau_h$ , where  $p_{\pm}^{(h)}(x, t)$ , h = 1, 2, are defined in the disjoint subsets  $\Omega_1$ ,  $\Omega_2$ , respectively.

The boundary condition at an ideal interface follows from the hyperbolic structure of eq. (13) by imposing that there is no singularity at the interface (alternatively, one can invoke steady-state conditions). To this purpose, instead of eq. (13), let us consider a mollified version of it, by defining a smooth velocity field  $b_{\varepsilon}(x)$ , which is  $C^k(\mathbb{R})$ , with  $k \geq 1$  with respect to x for any  $\varepsilon > 0$ , and such that, in the limit for  $\varepsilon \to 0$ , it reproduces the discontinuity in the lattice phase velocities

$$\lim_{\varepsilon \to 0} b_{\varepsilon}(x) = \begin{cases} b_1, & x \in \Omega_1, \\ b_2, & x \in \Omega_2, \end{cases}$$
(14)

and similarly for the transition rates  $\lambda_h$ , introducing a smooth field  $\lambda_{\varepsilon}(x)$ . With respect to this mollified description, eq. (13) becomes

$$\frac{\partial p_{\pm}(x,t)}{\partial t} = \mp \frac{\partial [b_{\varepsilon}(x)p_{\pm}(x,t)]}{\partial x} \mp \lambda_{\varepsilon}(x) \left[p_{+}(x,t) - p_{-}(x,t)\right].$$
(15)

Let  $x_0$  be the position of an ideal interface. Integrating eq. (15) in the interval  $[x_0 - \eta, x_0 + \eta]$ , where  $\eta > 0$  is a small parameter, and introducing the bounded quantities

$$Dp_{\max} = \max_{x \in [x_0 - \eta, x_0 + \eta]} \left| \frac{\partial p_{\pm}(x, t)}{\partial t} \right|,$$
  

$$\lambda_{\max} = \max_{x \in [x_0 - \eta, x_0 + \eta]} \lambda_{\varepsilon}(x), \qquad (16)$$
  

$$\Delta_{\max} = \max_{x \in [x_0 - \eta, x_0 + \eta]} |p_{+}(x, t) - p_{-}(x, t)|.$$

All these quantities are to be finite, at least for sufficiently long timescales. Consequently,

$$|b_{\varepsilon}(x_0+\eta) p_{\pm}(x_0+\eta,t) - b_{\varepsilon}(x_0-\eta) p_{\pm}(x_0-\eta,t)| \le 2\eta K,$$
(17)

where  $K = Dp_{\max} + \lambda_{\max} \Delta_{\max}$ . In the limit for  $\eta \to 0$  the condition

$$b_{\varepsilon}(x_0^-) p_{\pm}(x_0^-, t) = b_{\varepsilon}(x_0^+) p_{\pm}(x_0^+, t), \qquad (18)$$

is recovered. Taking the limit for  $\varepsilon \to 0$ , the velocity-based boundary condition follows,  $b_1 p_{\pm}^{(1)}(x_0, t) = b_2 p_{\pm}^{(2)}(x_0, t)$ , corresponding to eq. (5).

It is possible to provide a lattice dynamics-based analysis of the interfacial boundary conditions leading to eq. (5) generalizing the approach developed by Ovaskainen and Cornell [24] which derive the same boundary condition in Appendix A.1 Case A (in the case of pure spatial heterogeneity). In point of fact, in the Ovaskainen and Cornell paper, the symmetric case of an ideal interface (considered in the present work), corresponds to z = 0, and the quantities  $q_{\pm}$  used in their analysis are proportional to  $\delta_h$ , h = 1, 2.

Numerical experiments. – In point of fact, eq. (6) represents a change of paradigm with respect to the usual approach to boundary conditions applied at interfaces in the presence of diffusion, in which  $p^{(2)}/p^{(1)}|_{x=x_0}$  is assumed equal to the ratio of the diffusivities  $D_1/D_2$  [11,14–16]. Equation (5) finds its natural explanation in the stochastic models in which the finite value of the propagation velocities  $b_h$  is assumed, while it is "alien" to the classical parabolic approach. In this framework, the analysis of MuPh-LRW is a significant benchmark to test the importance of the physical assumptions underlying hyperbolic transport theories [23,26,27].

Direct numerical simulations of MuPh-LRW provides a clear answer to this question. Consider a MuPh-LRW on a closed domain  $x \in [-1, 1]$  equipped with zero-flux conditions at the endpoints. The interval [-1, 0) corresponds to the lattice phase "1", (0, 1] to the lattice phase "2", and the interface is located at  $x = x_0 = 0$ . In the simulations,  $\delta_1 = 1/N$ ,  $N_1 = N$  is the number of lattice sites in phase "1",  $\delta_2 = \delta_1/\alpha$ , where  $\alpha$  is an integer, so that  $N_2 = \alpha N$  is the number of sites of phase "2", while  $\tau_1 = 1$  and  $\tau_2$  freely varies. An ensemble of  $10^6$  particles is considered, initially located at the interface.

Figures 2 and 3 depict the comparison of the lattice simulations of MuPh-LRW with the results obtained by integrating the hyperbolic equations (1) for each phase and in each disjoint phase domain where the boundary conditions (5) have been applied at the interface x = 0. Figure 2 refers to  $\delta_2 = \delta_1/4$ ,  $\tau_2 = \tau_1$ , so that  $p^{(2)}/p^{(1)}|_{x=0} = 4$ , while the classical diffusive boundary condition provides  $p^{(2)}/p^{(1)} = 16$ . Figure 3 refers to  $\delta_2 = \delta_1/2$ ,  $\tau_2 = \tau_1/2$ , at which the hyperbolic theory predicts a smooth overall concentration profile across the interface as  $p^{(2)}/p^{(1)}|_{x=0} = 1$ , while the diffusive boundary condition implies a discontinuity  $p^{(2)}/p^{(1)}|_{x=0} = 2$ .

The lattice simulation results are accurately described by the hyperbolic hydrodynamic model, and the validity of the velocity-based interfacial condition (6), or eq. (5), is highlighted by the data depicted in fig. 4 referred to the



Fig. 2: Probability density function p(x,t) vs. x at several time instants for  $\delta_2 = \delta_1/4$ ,  $\tau_2 = \tau_1$ . Symbols ( $\circ$ ) are the results of lattice simulations, continuous lines the solutions of the corresponding hyperbolic model. Panel (a) refers to  $t = 2 \times 10^2$ , (b) to  $t = 10^3$ , (c) to  $t = 5 \times 10^3$ , (d) to  $t = 10^4$ .



Fig. 3: Same as in fig. 2 at  $\delta_2 = \delta_1/2$ ,  $\tau_2 = 1/2$ .



Fig. 4: Particle frequency  $p_1^*$  in phase "1" at steady state as a function of  $\tau_1/\tau_2$  in a MuPh-LRW closed cell  $x \in [-1, 1]$ at  $\delta_2 = \delta_1/2$ . Symbols are the results of lattice simulations, curve (a) corresponds to  $p_1^* = (b_2/b_1) p_2^*$ , curve (b) to  $p_1^* = (D_2/D_1) p_2^*$ .

particle fraction  $p_1^*$  at steady state in phase "1", obtained from lattice simulations, as a function of the ratio  $\tau_1/\tau_2$ , compared with the result deriving from eq. (6) and constrasted with the parabolic interpretation of the boundary conditions based on the ratio of the phase diffusivities. An important observation is related to the connection between the theory developed in this letter and the existing literature in the field, specifically the works [11–13]. Korabel and Barkai [11–13] apply the boundary condition based on the ratio of the diffusivities in the framework of anomalous diffusion problems, finding numerical confirmation of this via stochastic simulations of a Continuous Time Random Walk (CTRW) model. In point of fact, the results

ature in the field, specifically the works [11–13]. Korabel and Barkai [11–13] apply the boundary condition based on the ratio of the diffusivities in the framework of anomalous diffusion problems, finding numerical confirmation of this via stochastic simulations of a Continuous Time Random Walk (CTRW) model. In point of fact, the results presented in these articles are not in disagreement with the present theory and, in some sense, provide a further confirmation of it. This is because the authors consider a multiphase lattice structure possessing the same lattice spacing homogeneously throughout the two phases, and such that the phase heterogeneity is characterized by two different statistics of the hopping times in the two phases. Transferring this setting into a regular MuPh-LRW, this means that  $\delta_1 = \delta_2 = \delta$  while  $\tau_1 \neq \tau_2$ . Consequently,  $D_1/D_2 = \tau_2/\tau_1 = b_1/b_2$ , and therefore the ratio of the phase diffusivities coincides with the ratio of the phase velocities, so that the boundary condition used in [11-13]reduces to eq. (5).

Dispersion in a periodic multiphase lattice. -Once the qualitative and quantitative validity of the hyperbolic description and of the interfacial conditions arising from it has been assessed, it is possible to use this hydrodynamic model to investigate finer transport properties of MuPh-LRW. Specifically, we consider a dispersion experiment on a lattice composed by the periodic repetition of a multiphase unit cell as depicted in fig. 5. The unit lattice structure is the same used for the data in figs. 2 and 3, with physical length L = 2,  $L_1 = L_2 = 1$  and  $\delta_1 = 1/N$ , where  $N = N_1 = 100$ ,  $\tau_1 = 1$ ,  $\delta_2 = \delta_1/\alpha$  and  $\tau_2$  varies. By considering an ensemble of  $10^6$  particles initially located at  $z_0 = 0$  ( $x_0 = 0$ ), the first order moments (mean and mean square displacement) are estimated, and from their linear scalings with time t in the long-term regime, the value of the effective velocity  $V_{\text{eff}}$  and effective diffusivity  $D_{\text{eff}}$  (dispersion coefficient) obtained. From the simulations one obtains  $V_{\text{eff}} = 0$ , while the results for  $D_{\text{eff}}$ as a function of  $\tau_1/\tau_2$ , varying  $\delta_1/\delta_2$  are depicted in fig. 6.

These data should be compared with the long-term properties derived from the continuous hyperbolic model based on eq. (1) obtained from exact moment analysis [28]. In order to have a qualitative picture of the influence of the finite velocity assumption in the long-term hydrodynamic behavior of MuPh-LRW, we consider also the modeling of particle motion in terms of a Langevin equation driven by a Wiener process, and leading to a parabolic Fokker-Planck equation. Taking into account the nonlinear and discontinuous nature of the resulting Langevin equation, we consider the most general interpre-



Fig. 5: Schematic representation of a LRW in a periodic lattice structure possessing a multiphase unit periodicity cell.



Fig. 6: Dispersion coefficient  $D_{\text{eff}}/D_1$  for particle transport in a periodic multiphase lattice as a function of  $\tau_1/\tau_2$ . Symbols are the results of lattice simulations, solid lines are the predictions of homogenization theory applied to the hyperbolic transport model. Line (a) and ( $\Box$ ) refers to  $\delta_1/\delta_2 = 1$ , line (b) and ( $\blacksquare$ ) to  $\delta_1/\delta_2 = 2$ , line (c) and ( $\circ$ ) to  $\delta_1/\delta_2 = 3$ , line (d) and ( $\bullet$ ) to  $\delta_1/\delta_2 = 4$ , line (e) and ( $\triangle$ ) to  $\delta_1/\delta_2 = 5$ .

tation of it, namely  $dx(t) = \sqrt{2D(x(t))} *_{\lambda} dw(t)$ , where D(x) = D(x + L) is the discontinuous and spatially periodic diffusivity profile attaining the values  $D_h$  in each lattice phase, dw(t) the increment of a Wiener process in the time interval dt and " $*_{\lambda}$ " indicates that the  $\lambda$ -calculus,  $\lambda \in [0, 1]$ , has been chosen in the definition of the stochastic Stieltjes integrals ( $\lambda = 0, 1/2, 1$  correspond to the Ito, Stratonovich and Hänggi-Klimontovich interpretation, respectively) [29]. A detailed account of the exact homogenization analysis of the different hydrodynamic models can be found in [28]. The final result (for  $L_1 = L_2 = 1$ ) is

$$\frac{1}{D_{\text{eff}}} = \frac{1}{2} \left( \frac{1}{b_1} + \frac{1}{b_2} \right) \left( \frac{1}{b_1 \tau_1} + \frac{1}{b_2 \tau_2} \right)$$
(19)

for the hyperbolic model, and

$$\frac{1}{D_{\text{eff}}} = \frac{1}{4} \left( \frac{1}{D_1^{1-\lambda}} + \frac{1}{D_2^{1-\lambda}} \right) \left( \frac{1}{D_1^{\lambda}} + \frac{1}{D_2^{\lambda}} \right)$$
(20)

for the Langevin-Wiener model associated with a  $\lambda$ -interpretation of the stochastic integrals. The data depicted in fig. 6 clearly indicate that the hyperbolic transport model accurately accounts for the dispersion properties in a multiphase lattice. Conversely, even keeping  $\lambda$  as an adjustable parameter, it is impossible for any Langevin-Wiener model of MuPh-LRW diffusion to provide a quantitative estimate of the long-term dispersion properties. This claim is supported by the data depicted in



Fig. 7:  $D_{\text{eff}}/D_1 vs. (\tau_1/\tau_2)^{1/2}$  for dispersion in a periodic multiphase lattice for a fixed ratio  $D_1/D_2$ . Symbols are the results of lattice simulations, solid lines (a) and (b) are the predictions of the hyperbolic transport model eq. (19). Line (a) and ( $\Box$ ) refer to  $D_1/D_2 = 1$ , line (b) and ( $\circ$ ) to  $D_1/D_2 = 4$ . The horizontal lines represent the lower and upper bounds in the predictions of the parabolic transport model obtained by varying  $\lambda$ : line (c) refers to  $D_1/D_2 = 1$ , lines (d) and (e) to  $D_1/D_2 = 4$ .

fig. 7. These data refer to the effective diffusion coefficient in a periodic multiphase lattice at  $\delta_2 = \delta_1/\gamma\xi$ ,  $\tau_2 = \tau_1/\xi^2$ by varying the parameters  $\gamma$ , and  $\xi$ . For fixed values of  $\gamma$ , the ratio  $D_1/D_2 = \gamma^2$  is constant. From eq. (20) it follows that any Langevin-Wiener model of particle transport would predict a constant value of  $D_{\rm eff}$  independently of the value of  $\xi$ . Conversely, the hyperbolic model based on eq. (1) predicts a value of  $D_{\rm eff}/D_1$  that depends continuously on the ratio  $\tau_1/\tau_2 = \xi^2$  for fixed  $\gamma$ . Lattice simulation results depicted in fig. 7 support the latter prediction of the hyperbolic hydrodynamic model. In the case  $D_1/D_2 = 1$ , one has  $D_{\rm eff}/D_1 = 1$  from the parabolic model, independently of  $\lambda$  (line (c) in fig. 7), while in general  $D_{\rm eff}/D_1$  in parabolic Langevin-Wiener models is lower- and upper-bounded by the values attained at  $\lambda = 0$ and  $\lambda = 1/2$ .

This result indicates that the hyperbolic hydrodynamic model not only provides a more quantitatively consistent alternative to parabolic models for describing LRW at short timescales, as addressed in [21], but it is the only continuous model deriving from a continuous stochastic description of particle transport constistent with longterm dispersion data in multiphase periodic lattices.

Reversing the latter argument, it implies that the assumption of finite-time propagation velocity is a fundamental prerequisite in order to predict correctly both the long-time dispersion properties in infinite multiphase lattices and the equilibrium properties in closed multiphase cells.

The latter observation opens up interesting perspectives in the hydrodynamic modeling of particle systems based on the fundamental assumption of finite propagation velocity. This observation finds a significant experimental confirmation in the ubiquitous evidence of ballistic transport at short timescales both in micro- and nanostructures [30–32], and sheds new light on the conceptual relevance in non-equilibrium statistical physics of stochastic approaches deeply grounded on the "weak relativistic principle" of finite propagation velocity. The same approach can be extended to electron-transport in periodic lattices, in order to determine the effective electron mass in all the solid-state systems in which experimental evidence suggests an effective relativistic constraint associated with a bounded velocity of carrier particles [33,34].

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