Random walks in random stochastic environments

Miguel Ángel García-March,[1,*] Gerald J. Lapeyre Jr.,[2] Pietro Massignan,[1] and Maciej Lewenstein[1,3]

[1] *ICFO – Institut de Ciències Fotòniques, Castelldefels (Barcelona) 08860, Spain*
[2] *IDAEA – Institute of Environmental Assessment and Water Research, c/ Jordi Girona, 18-26, Barcelona 08034, Spain*
[3] *ICREA – Institució Catalna de Recerca i Estudis Avançats, Passeig Lluís Companys, 23 Barcelona 08010, Spain*

I. INTRODUCTION

Recently, there has been considerable interest in random walk models in disordered media characterized by random diffusivity (cf.[1,2] and references therein). Such models lead in a natural way to the appearance of anomalous subdiffusive behavior, lack of ergodicity, aging and similar effects. For these reasons they are suitable to model various complex phenomena, such as diffusion of enzymes or receptors on a cell surface, observed using single particle imaging in *in vivo*[2], or an impurity strongly interacting with a condense matter system.

The main aim of the present project is to formulate and investigate a family of "microscopic" models of a random walk in a random stochastic medium. The dynamics of the medium will be described by a kinetic process that depends on the location of the walker (or, in more general cases, on the walker's history). At every moment, the dynamics of the walker will depend on the configuration of the environment. Both dependences will be assumed to be local, i.e. they involve only the vicinity of the walker's locations. By appropriately modeling these couplings we expect to formulate new families of many-body stochastic models with a moving impurity, capable of reproducing results for random walks in quenched disorder (if the environment dynamics is ultra slow), and much more. As an example we discuss here a paradigm model of a random walker in the environment described by Glauber's famous kinetic Ising model[3].

II. EXAMPLE

Let us consider systems described by classical Hamiltonians $H(\sigma)$. We are interested in Hamiltonians following Markovian dynamics towards equilibrium. For concreteness, we consider σ to be the N-dimensional Ising vectors $\sigma = (\sigma_1, \ldots, \sigma_N)$, with Ising variables $\sigma_i = \pm 1$. Let us denote the conditional probability of reaching state σ at time t when the system is initially in the state σ_0 as $P(\sigma, t|\sigma_0, 0)$ (of course $P(\sigma, 0|\sigma_0, 0) = \delta_{\sigma,\sigma_0}$). We use the shorthand notation $P(\sigma, t)$. Then, the dynamical evolution is given by

$$\dot{P}(\sigma,t) = \sum_{\sigma'} [w(\sigma' \to \sigma) P(\sigma', t) - w(\sigma \to \sigma') P(\sigma, t)] , \quad (1)$$

where the transition rates $w(\sigma' \to \sigma)$ are the probability per unit time for the transition from configuration σ' to σ. It is natural to assume the detailed balance condition (DBC), that is, to impose that

$$w(\sigma' \to \sigma) P_{\rm eq}(\sigma') = w(\sigma \to \sigma') P_{\rm eq}(\sigma) \quad (2)$$

with $P_{\rm eq}(\sigma) = P(\sigma, t \to \infty)$.

Let us consider the ferromagnetic Ising model, $H(\sigma) = -J \sum_i^{N-1} \sigma_i \sigma_{i+1}$, $J > 0$. The probability distribution at equilibrium is

$$P_{\rm eq}(\sigma) = \frac{1}{Z_N} e^{-\beta H(\sigma)}, \quad (3)$$

with partition function $Z_N = 2^N (\cosh^N \beta J + \sinh^N \beta J)$. We restrict the dynamics to single spin flips, $\sigma' = D_i \sigma$. That is, a configuration σ is only connected to other configurations by this process and the transition rates are of the form $w(D_i\sigma \to \sigma)$. With these assumptions Eq. (1) becomes

$$\dot{P}(\sigma,t) = \sum_{i=1}^{N} [w(D_i\sigma \to \sigma) P(D_i\sigma, t) - w(\sigma \to D_i\sigma) P(\sigma, t)] .$$

Under these conditions a conventional form for the transition rates is[3]

$$w(D_i\sigma \to \sigma) = \Gamma \left[1 - \frac{1}{2} \tanh [2\beta J] \, \sigma_i (\sigma_{i-1} + \sigma_{i+1}) \right], \quad (4)$$

where the parameter Γ is the time scale at which the transitions occur.

Let us make the Ansatz $P(\sigma, t) = \sqrt{P_{\rm eq}(\sigma)} \phi(\sigma, t)$, with $\phi(\sigma, t)$ to be determined. For our model Hamiltonian this reads $P(\sigma, t) = \exp [\beta J \sum_i \sigma_i \sigma_{i+1}/2] \, \phi(\sigma, t)$. Then, from Eq. (1) we have

$$\dot{\phi}(\sigma,t) = \sum_{\sigma'} \Big\{ P_{\rm eq}^{-1/2}(\sigma) w(\sigma' \to \sigma) P_{\rm eq}^{1/2}(\sigma') - P_{\rm eq}^{-1/2}(\sigma') \sum_{\sigma''} w(\sigma' \to \sigma'') P_{\rm eq}^{1/2}(\sigma') \delta_{\sigma\sigma'} \Big\} \phi(\sigma', t),$$

which can be written as a Schrödinger equation $\dot{\phi}(\sigma, t) = H\phi(\sigma, t)$. For Glauber's case [transition rates given by Eq. (4)] one has

$$H(\gamma) = -\Gamma \sum_i \left\{ [A(\gamma) - B(\gamma) \sigma_{i-1}^z \sigma_{i+1}^z] \sigma_i^x - [1 - \tfrac{\gamma}{2} \sigma_i^z (\sigma_{i-1}^z + \sigma_{i+1}^z)] \right\},$$

with $\gamma = \tanh 2\beta J$, σ^z and σ^x the Pauli matrices, $A(\gamma) = \gamma^2/[(2(1 - \sqrt{1-\gamma^2})]$ and $B(\gamma) = 1 - A(\gamma)$. Hamiltonian (5) can be diagonalized by a Jordan-Wigner transformation.

III. CURRENT PROJECT

Our aim is to analyze systems derived from this model in the presence of an impurity. In these models, when the impurity occupies site m, the system's coefficients are changed in some way. The following models show this behavior:

- The energy is increased locally by $\bar{h}$ at the position of the impurity. That is

$$H = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} + H_{\mathrm{I-bath}} \tag{5}$$

  with $H_{\mathrm{I-bath}} = \sum_i^N h_i^m$ with $h_i^m = \bar{h}\delta_{im}\sigma_i$ (site impurity) or $h_i^m = \bar{h}(\delta_{i,m}\sigma_i + \delta_{i-1,m}\sigma_{i-1})$ (link impurity). In the first case, when the impurity is at site m, if the spin at that site is $+1$, energy is increased by $\bar{h}$, and is decreased by $\bar{h}$ if it is -1.

- The interaction energy depends on the position of the impurity. Then,

$$H = -\sum_{i=1}^{N-1} J_i^m \sigma_i \sigma_{i+1} \tag{6}$$

  with $J_i^m = J + \chi(\delta_{i,m} + \delta_{i+1,m})$.

- Spread the effect of the impurity over a range of sites. For example, Hamiltonian (6) with $J_i^m = J + \sum_{j,\langle j,m\rangle} \chi\delta_{im}$.

Additionally, one can consider that the impurity may be subject to an external potential $V(m)$. This potential can be parabolic or a random potential, that is, something which forces the impurity to be localized in equilibrium. The configuration of the system of spins plus impurity is (σ, m), with Ising variables $\sigma_i = \pm 1$, $i = 1, \ldots, N$ and $m \in 1, \ldots, N$ being the position of the impurity. One can write a Master equation for this system as

$$\begin{aligned}\dot{P}(\sigma,m,t) = &\textstyle\sum_i [w(D_i\sigma,\sigma)P(D_i\sigma,t) - w(\sigma,D_i\sigma)P(\sigma,t)] \\ &+ [W(m+1,m)P(m+1,t) + W(m-1,m)P(m-1,t) \\ &- W(m,m+1)P(m,t) - W(m,m-1)P(m,t)]\,,\end{aligned}$$

where the transition rates $w(D_i\sigma,\sigma)$ do not change the position of the impurity and the transition rates $W(m',m)$ stand for the probability per unit time that the impurity changes position from m' to m. It should conserve probability, be local, and obey DBC. The probabilities at equilibrium are in general

$$P_{\mathrm{eq}} = \frac{1}{Z}\exp[-\beta H(\sigma,m)]. \tag{7}$$

However, in equilibrium the impurity may be fully delocalized for those Hamiltonians which do not break translational symmetry for the impurity.

For Hamiltonian (6) one can go a bit further. The transition rates can be generalized from Glauber's to $1 - \tanh[2\beta J_i^m]\sigma_i(\sigma_{i-1}+\sigma_{i+1})$ and the Master equation can be written as

$$\begin{aligned}\dot{P}(\sigma,m,t) = \Gamma \sum_i \Big[&[D_i - 1](1 - \frac{1}{2}\tanh 2\beta J_i^m h_i P(\sigma,m,t)\Big] \\ &+ \alpha \exp[\chi\sigma_{m+1}(\sigma_m + \sigma_{m+2})P(\sigma,m+1,t)] \\ &+ \alpha \exp[\chi\sigma_{m-1}(\sigma_m + \sigma_{m-2})P(\sigma,m-1,t)] \\ &- 2\alpha \exp[-\chi\sigma_m(\sigma_{m-1} + \sigma_{m+1})P(\sigma,m,t)]\end{aligned} \tag{8}$$

with $h_i = \sigma_i(\sigma_{i-1}+\sigma_{i+1})$ and where α and Γ allow for different time scales in both types of transitions. Our goals are: i) find models such as those described above that are exactly solvable in 1D; ii) Perform numerical studies of these kind of models with Monte Carlo and Tensor Network States methods; iii) Apply them to various realistic scenarios, as the aforementioned biological systems or to exotic applications like a classical model for gravity.

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* miguel.garcia-march@icfo.es

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