

Hopping diffusion of two coupled particles in the random trap model

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We show that the hopping dynamics of two strongly connected particles can be mapped exactly to single particle dynamics. In this way we are able to calculate the exact asymptotic diffusion coefficient of two connected particles on a linear chain in the random trap model. In particular we calculate the diffusion coefficient for exponentially distributed site energies and show that there exists a critical temperature below which a subdiffusive behavior appears. It turns out that this critical temperature is twice higher than the critical temperature in the single particle case [S. Havlin, B. L. Trus, and G. H. Weiss, *J. Phys. A: Math. Gen.* **19**, L817 (1986)].

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I. INTRODUCTION

Hopping diffusion of classical particles in quenched random media has been the subject of many investigations in the past years (see for reviews [1–5]). In most of these investigations the random medium was simplified by a so called random energy model where the underlying structure is translationally invariant and the disorder is introduced by defining disordered jump rates between the lattice sites chosen randomly from a given distribution (examples are the random trap model, the random barrier model, etc.). The asymptotic behavior of single particle diffusion in such translationally invariant disorder models is at least in one dimensional cases completely understood [6]. However, the description of the dynamics of interacting particles such as the dynamics of lattice gases [7,8], single file diffusion [9], polymer chains [10–15], etc. even in lattices with uniform transition rates is much more complex and is the subject of many recent and current investigations. The subject of this paper is the diffusion of two coupled particles on a one dimensional lattice with random site energies. A model where the particles are connected by a attracting harmonic potential was investigated recently [16]. This is apparently the simplest model of coupled hopping particles and can be seen as a starting point of understanding the diffusion of polymer chains in random media. The diffusion of polymer chains in random media is one of the most fundamental and important quantities and has a broad application in material, biological and physical science and also in industrial purposes.

In the following section we will introduce the model. In Sec. III we derive the exact diffusion coefficient of the center of mass by mapping the dynamics of the two coupled particles into a single particle case. In the last section we conclude and discuss the case of longer chains.

II. MODEL

Consider two connected particles which perform continuous time random walk (CTRW) on a one dimensional lattice

in the following way. Each particle has its own clock after which it jumps to a neighboring site under the condition that the distance between the two particles is no longer than one lattice site (see Fig. 1). The particles can be either at the same site or sitting on two neighboring sites. Each lattice site i corresponds to an energy trap E_i , where the particle is trapped and try to release at each time unit (random trap model). Therefore the waiting time distribution of the particle at site i is an exponential function [17] which depends on the depth of the trap at this site:

$$\psi_i(t) = \frac{1}{\tau_i} e^{-t/\tau_i}, \quad (1)$$

where τ_i is the mean waiting time of a particle at site i . The exponential factor represent the probability that the particle has not yet jumped until time t and the prefactor is the jump rate of the particle. The jump rate Γ_i depends on temperature and on the energy trap at site i ,

$$\Gamma_i = \Gamma_0 e^{-E_i/k_B T}, \quad (2)$$

where Γ_0 is the attempt frequency, k_B is the Boltzmann factor and T the temperature of the system.

To be precise the jump direction of a particle depends on the position of the two particles. If the particle performing the jump is at site i and the other particle at site j than the jump rate from site i to a nearest neighboring site f is given by

$$\Gamma_{i,f} = \Gamma_0 \exp[-\beta V_{i,f}(i,j)], \quad (3)$$

where $\beta = 1/(k_B T)$ and

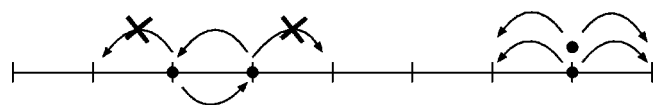


FIG. 1. The allowed jumps of two connected particles. The distance between the two particles must not be more than one lattice site.

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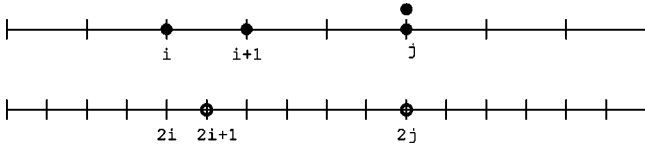


FIG. 2. Mapping to the single particle case by considering the center of mass of the two connected particles. The odd or even sites represent the configurations where the particles are sitting on neighboring sites or at the same position, respectively.

$$V_{i,f}(i,j) = \begin{cases} \infty & \text{if } |j-f| > 1, \\ E_i & \text{if } j=f, \\ E_i - \frac{1}{\beta} \ln\left(\frac{1}{2}\right) & \text{if } i=j. \end{cases} \quad (4)$$

III. MAPPING TO A SINGLE PARTICLE PICTURE AND EXACT DIFFUSION COEFFICIENT OF THE CENTER OF MASS

Now consider the motion of the center of mass of two connected particles. Due to the independent jumps of the particles the motion of the center of mass can be represented by an uncorrelated hopping of a single particle on a chain with additional sites in between the sites of the previous chain (see Fig. 2).

We number the sites in the chain of the center of mass picture in a way where the center of mass is on an even or odd site when the two particles are at the same position or at neighboring positions, respectively (see Fig. 2). The jump rates in the center of mass picture are related to the jump rates of the original model in the following way:

$$r_{2i} = \Gamma_i, \quad l_{2i+1} = \Gamma_i, \quad r_{2i+1} = \Gamma_i, \quad l_{2i+1} = \Gamma_{i+1}, \quad (5)$$

where r_n , l_n are the jump rate of the center of mass to the right and to the left, respectively.

The master equation which gives the time evolution of the conditional probability $P_n(t)$ to find the center of mass at the site n at time t if it was at time 0 at site 0 can be written as

$$\frac{d}{dt} P_n(t) = r_{n-1} P_{n-1} + l_{n+1} P_{n+1} - (r_n + l_n) P_n. \quad (6)$$

A numerical solution and the comparison with computer simulations are given in Fig. 3. The dynamics of the connected particles are mapped to the dynamics of one particle in a different energy landscape which we will construct later on. In this way we can use the exact result of the diffusion coefficient of a single particle in a one dimensional translational invariant lattice with arbitrary quenched jump rates [18–20]

$$D = \left\{ \frac{1}{r_n P_n^{\text{eq}}} \right\}^{-1}, \quad (7)$$

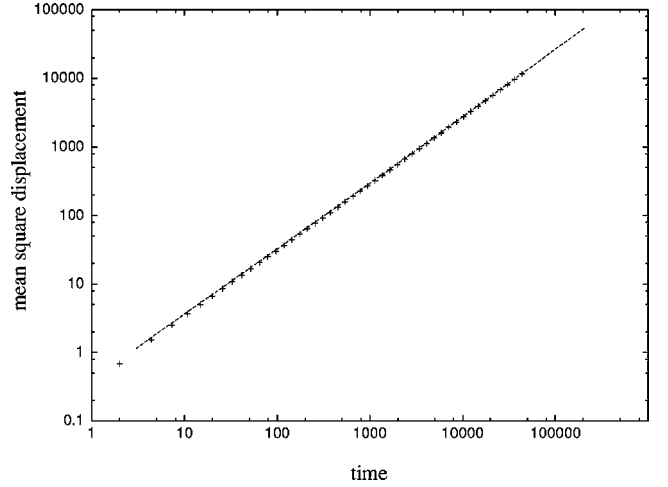


FIG. 3. Mean square displacement (arbitrary units) versus time (arbitrary units) in a double logarithmic plot where numerical results of the master equation (6) (dashed line) are compared to the Monte Carlo simulations (+ signs) for an exponentially distributed energy level at $T=3$ and mean energy level $\sigma=1$.

where the curly brackets indicate the disorder average and P_n^{eq} represents the equilibrium occupation probability at site n and it is given by

$$P_n^{\text{eq}} = \frac{\exp(\beta \epsilon_n)}{Z}. \quad (8)$$

$Z = \{\exp(\beta \epsilon_n)\}$ is the partition function and ϵ_n is the positive counted energy levels in the energy landscape of the center of mass which can be constructed recursively in the following way (see Fig. 4):

$$\epsilon_{2i} = \epsilon_{2i-1} - E_i + E_{i+1}, \quad (9)$$

$$\epsilon_{2i+1} = \epsilon_{2i} - E_i + E_{i+1}. \quad (10)$$

Solving these recursive relations and setting $\epsilon_1 = E_1 = 0$ we find a simple relation to the energy levels in the original random trap model

$$\epsilon_{2i} = E_i + E_{i+1}, \quad (11)$$

$$\epsilon_{2i+1} = 2E_{i+1}. \quad (12)$$

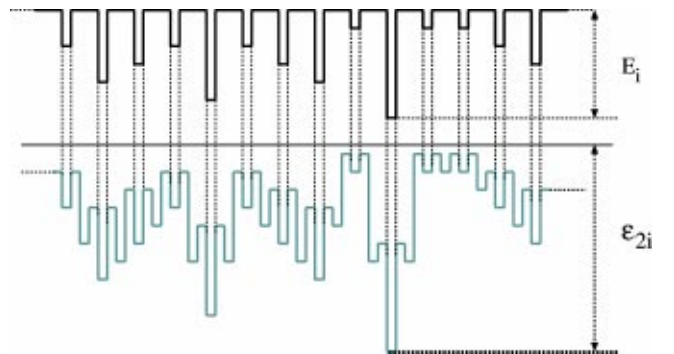


FIG. 4. The construction of the energy landscape in the center of mass picture.

We are interested in dynamics at equilibrium where the detailed balance condition has to be valid and this can be proved

$$\begin{aligned}
 P_{2i}^{\text{eq}} r_{2i} &= \frac{1}{Z} e^{\beta(E_i + E_{i+1})} e^{-\beta E_i} \\
 &= \frac{1}{Z} e^{\beta E_{i+1}} \\
 &= \frac{1}{Z} e^{2\beta E_{i+1}} e^{-\beta E_{i+1}} \\
 &= P_{2i+1}^{\text{eq}} l_{2i+1}.
 \end{aligned} \tag{13}$$

The diffusion coefficient now takes the following form:

$$D = a^2 \{e^{\beta \epsilon}\}_{\epsilon}^{-1} \{e^{-\beta E}\}_E^{-1}. \tag{14}$$

The first disorder average on the right side is the inverse partition function and the second is the disorder average over the “weighted” jump rates $Z r_n P_n^{\text{eq}}$ which are simplified by the detailed balance relation (13). The use of Eqs. (11) and (12) leads to the following form of the diffusion coefficient:

$$D = a^2 \left[\frac{1}{2} \{e^{\beta(E+E')}\}_{E,E'} + \frac{1}{2} \{e^{2\beta E}\}_E \right]^{-1} \{e^{-\beta E}\}_E^{-1},$$

where the indices at the curly brackets indicate the parameter of the disorder average. The first disorder average is simply a double integration over the distribution of the energies.

$$D = \begin{cases} \frac{1}{2} (1 + \beta\sigma) [(1 - 2\beta\sigma)^{-1} + (1 - \beta\sigma)^{-2}]^{-1} & k_B T > 2\sigma \\ 0 & k_B T < 2\sigma. \end{cases} \tag{16}$$

In Fig. 5 one can see the good agreement of the result of Eq. (16) and Monte Carlo simulations. The deviation of the last points are due to the very slow dynamics of the two coupled particles. At low temperatures the linear regime of the mean square displacement is reached after a very long time.

V. DISCUSSION

We have seen that the hopping dynamics of two connected particles as modeled in Sec. II on a linear chain with arbitrary jump rates can be reduced into single particle dynamics by considering the dynamics of the center of mass. This mapping allows the derivation of the exact diffusion coefficient. In the case of exponential distributed energy traps there occurs a dynamic phase transition such as in the single particle case where the critical temperature is a factor of two smaller. In the model considered in this paper, the center of mass is representing directly the two configura-

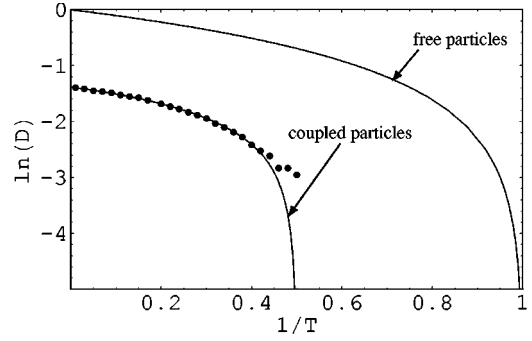


FIG. 5. Comparison of the theory (solid line) and Monte Carlo simulations (dots) in an Arrhenius plot where the inverse temperature (arbitrary units) is plotted versus the logarithm of the diffusion coefficient (arbitrary units). The case of single (or free) particle diffusion is also compared to the case of the coupled particles. The energy levels are distributed randomly from an exponential distribution.

IV. EXAMPLE: EXPONENTIAL DISTRIBUTED ENERGY TRAPS

In this section we consider a disorder model where the traps are distributed by

$$\rho(E) = \frac{1}{\sigma} \exp\left(-\frac{E}{\sigma}\right), \tag{15}$$

where σ is the mean energy.

In this model it is shown that the single particle diffusion exhibits a dynamical phase transition at $T_c = \sigma/k_B T$ [21]. The diffusion coefficient in the two particle case exhibits also a dynamical phase transition but at a higher temperature:

tional states of the connected particles. One configuration is where both particles are sitting at the same site and the other is where the particles are sitting on neighboring sites. Due to this fact the dynamics of the two connected particles could be described fully by the dynamics of the center of mass. This is not possible anymore if one considers longer chains, where the configurational state of the chain is not represented by the center of mass in a unique way. Here other quantities should be considered which can represent all the states. And the “multistate random walk” of this quantity can then be projected to the center of mass in order to find its diffusion coefficient.

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