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Normal and anomalous diffusion of Brownian particles on disordered potentials

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HIGHLIGHTS

- A model of Brownian particles on disordered potentials exhibiting a transition from normal to anomalous subdiffusion is introduced.
- We obtain the exact effective diffusion coefficient, which allows to exactly determine critical temperature.
- The subdiffusive phase is analytically treated by approximating it by the random trap model.
- The diffusion exponents are obtained approximately in a closed form.

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ABSTRACT

In this work we study the transition from normal to anomalous diffusion of Brownian particles on disordered potentials. The potential model consists of a series of “potential hills” (defined on a unit cell of constant length) whose heights are chosen randomly from a given distribution. We calculate the exact expression for the diffusion coefficient in the case of uncorrelated potentials for arbitrary distributions. We show that when the potential heights have a Gaussian distribution (with zero mean and a finite variance) the diffusion of the particles is always normal. In contrast, when the distribution of the potential heights is exponentially distributed the diffusion coefficient vanishes when the system is placed below a critical temperature. We calculate analytically the diffusion exponent for the anomalous (subdiffusive) phase by using the so-called “random trap model”. Our predictions are tested by means of Langevin simulations obtaining good agreement within the accuracy of our numerical calculations.

1. Introduction

Transport of classical overdamped particles in random media has been intensively studied due to its relevance in several physical systems [1]. Several models of transport in disordered media have been introduced in order to understand the underlying mechanisms originating the observed phenomenology [1,2]. Some models exhibiting anomalous diffusion and transport are for example, the diffusion of particles on fractal geometry [3], the fractional Brownian motion [3], the single file diffusion of Brownian particles [4], particle systems with highly non-Markovian noise sources [5], diffusion of particles in magnetic traps [6], diffusion of deterministic particles in disordered media [7,8] or the diffusion of interacting particles [9].

Depending on the model type, the system can exhibit normal or anomalous transport accompanied with normal or anomalous diffusion. For example, in a recent work, it has been shown that a system of overdamped particles, on a random Gaussian potential with decaying correlations, the unbiased diffusion of particles is asymptotically normal [10]. A similar

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result has also be proved for uniformly bounded disordered potentials with decaying correlations in Ref. [11]. Particularly some attention has been addressed to models which exhibit a transition from normal to anomalous diffusion as a function of the temperature. A simplified model showing this feature is the so-called random trap model [12]. In this model the phase space consists of a "chain" of traps, indexed by $i \in \mathbb{Z}$ with depth ΔE_i. The time that a particle spent inside a trap has a distribution whose first moment diverges at a critical temperature $T_c > 0$. This result follows from the statistical properties of the energy depths ΔE_i with exponential distribution. Another model of Brownian particles with continuous disorder exhibiting a dynamical transition at a finite temperature consists of an ensemble of particles on a Gaussian squared potential [13].

In this work we study the particle–polymer model characterized by a continuous dynamics with discrete disorder [7,8,14,11]. We show that this kind of models, which can be considered in the middle between the random trap models (having discrete dynamics) and models with continuous disorder and continuous dynamics, is able to exhibit a temperature-dependent transition from anomalous to normal diffusion. The particle–polymer model consists of an ensemble of Brownian particles interacting with a random polymer. The polymer is built up by concatenating at random (by means of some stochastic process) monomers of constant length which can be taken from a finite or infinite set of monomer types. The interaction of a given particle with the monomers defines the potential profile acting on the particle in a specific unit cell. When the interaction is short-ranged we can think of this model as an ensemble of particles moving on a series of tracks, each track having a fixed random potential profile. Based on the theory developed in Ref. [14], we show that when the potential profile has barrier heights with normal distribution, the diffusion is always normal. In contrast, when the distribution of the potential barrier height is exponential, we show that there is a finite temperature T_c at which the system transits from normal to anomalous diffusion. We use the random trap model to approximate the behavior of the system in order to obtain an analytical expression for the diffusion exponent in the anomalous (subdiffusive) phase.

This work is organized as follows. In Section 2 we introduce the model of study and review some results already known for the system. In Section 3 we calculate the diffusion coefficient for the system by means of the Einstein relation which is known to be valid for our model. We also calculate explicitly the diffusion coefficient for the particles on potentials with Gaussian or exponential height distributions. We show that in the last case the diffusion coefficient is zero below a critical temperature. In Section 4 we study the diffusivity for potential heights exponentially distributed and temperature below the critical one. Since in this case the diffusion coefficient is zero the system exhibits anomalous subdiffusion. We implement what we call the "random trap" approximation. This approximation is based on identifying the waiting time distribution for the random trap model with the distribution of the mean first passage time induced by the disorder. This method allows us to obtain a good approximation for the diffusion exponent for the subdiffusive anomalous phase. We compare all the predictions made for this system against numerical simulations. Finally in Section 5 we give the main conclusions of our work.

2. The model

The particle–polymer model for transport in disordered media has been put forward in Ref. [7]. This model consists of an ensemble of non-interacting overdamped particles sliding over a 1D substrate. The substrate is modeled as a series of unit cells of constant length, called monomers if the substrate is interpreted as a polymer, with which the particles are interacting. This model mimics, in some sense, the motion of a given protein along a biological "disordered" polymer such as the DNA. The motion of a given particle along the referred substrate is ruled by the stochastic differential equation,

$$\gamma \, \mathrm{d}X_t = (f(X_t) + F)\, \mathrm{d}t + \varrho_0 \mathrm{d}W_t. \tag{1}$$

Here X_t represents the particle position at a time t, $f(x)$ is the negative of the gradient of the potential $V(x)$, which is the potential induced by the particle–polymer interaction and W_t is a standard Wiener process. The constants ϱ_0^2, F and γ are the noise intensity, the external driving force, and the friction coefficient, respectively. According to the fluctuation–dissipation theorem $\varrho_0^2 = 2\gamma\beta^{-1}$, where β, as usual, stands for the inverse temperature times the Boltzmann constant, $\beta = 1/k_B T$.

The interaction of the particle with the polymer specifies the potential profile seen by the particle when it is located at a specific monomer. If the particle–polymer interaction is short-ranged we can assume that the potential profile acting on the particle at a given monomer is defined exclusively by the monomer type at which the particle is located. Let $\mathbf{a} := (\dots, a_{-1}, a_0, a_1, \dots)$ be a specific realization of the random polymer, where a_j is the monomer type at the jth unit cell. The variable a_j can be interpreted as a random variable defining the interaction with the particle or the properties of the potential profile if the interaction is short-ranged. Thus, in this latter case, we can think of the potential $V(x)$ as a function of both the particle position x and the random variable a_n, where n is an index identifying the unit cell at which the particle is located. If the particle is located at the nth unit cell, then its position can be written as $x = nL + y$, where L is the length of the unit cell and y is the relative position of the particle in the monomer. Thus, the potential $V(x)$ can be written as a function ψ of two variables: the relative position y and the random monomer type, $V(x) = \psi(y, a_n)$. This model for disordered media was first studied in absence of noise in Ref. [7] where the authors showed that the particle current and the effective diffusion coefficient can be known exactly for a large class of disordered potentials. Later on, in Ref. [14] it was shown that the particle current and diffusion coefficient can still be exactly expressed in terms of quadratures. However in Ref. [14] the author was mainly interested in the case of biased transport, and, in fact, no formula for the diffusion coefficient in absence of driven force was found. Here we will explore the unbiased diffusion based on the findings of Ref. [14].