SUBDIFFUSIVE TRANSPORT IN MODEL DISORDERED MEDIA*

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We study the transport properties of two models of disordered media. In both cases we consider the motion of a particle which is not in thermal equilibrium with the environment. The first example is a hopping process in a one-dimensional lattice with random spacing, the second one is a random telegraph process in a random potential. We show, by computing the average stationary flux for a finite segment of the system, that the transport is subdiffusive if the temperature of the particle is lower than the temperature of the medium.

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1. Introduction

The diffusion of a particle among random scatterers or its motion in a static random potential has been the subject of many works (see a review in

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[1]). As it is now well known, it can lead to an abnormal diffusive behavior, either subdiffusive or surdiffusive, depending on the statistics of the potential and of the precise rules for the coupling of the particle to the external bath, and it seems rather difficult to find general reasons for a given behavior. This behavior is often characterized by the mean square displacement of the particle, which varies as the square root of time for normal diffusion. Another quantity of interest, however, is the transmission flux of a particle in a random potential in an interval of length L. The normal diffusive behavior for the transmission probability (*i.e.* the probability that the particle released at the extremity 0 of the interval is transmitted through the whole interval) is $O(L^{-1})$ for large L: this is the classical result obtained for a Brownian particle. It was proved that a short range spatial correlation between the values of the potential can lead to a superdiffusive behaviour: the transmission probability is then $O(L^{-1/2})$.

Here we investigate two different mechanisms that can produce a subdiffusive behavior for the flux. The first one is a hopping process on a one-dimensional lattice with random spacing: this spacing and the transition rate for hopping obey exponential laws, the exponent constants corresponding to the "temperatures" of the lattice and of the particle, respectively. The trajectories, the mean square displacement and the average transmission flux are studied; it is even possible to compute the distribution of the probability current. All these quantities depend critically on the ratio of the exponent constants, and the transport is shown to be subdiffusive if the "temperature" of the particle is lower than the temperature of the medium.

The same conclusion holds for our second model, which considers a particle moving with constant absolute velocity v on a line, but changing the sign of its velocity with a space dependent transition rate which represents its interaction with an inhomogeneous stochastic medium. In this model, we assume that the particle reaches a thermal equilibrium at inverse temperature β in a potential created by the environment, but due to the randomness of this environment, the potential is itself stochastic and is controlled by a different inverse temperature β'. We observe a phase transition at $\beta = \beta'$. For $\beta' > \beta$, the flux has a normal diffusive behavior, whereas it has a subdiffusive behavior for $\beta' < \beta$.

2. Hopping process in a one-dimensional lattice with random spacing

2.1. The model

Consider a particle performing random walk on the sites of a linear chain, where the intersite distances are independent random variables distributed according to a given probability distribution $\mu(l_j)$ (l_j is the distance between the j-th and $j+1$-th sites). The hopping process of a particle on that chain is characterized by the set of the nearest-neighbor transition rates $\{\Gamma_{j,j+1}\}$, where $\Gamma_{j,j+1}$ is the rate at which particle jumps from the site j to the site $j+1$, and is described by the following master equation

$$\frac{dP(j,t)}{dt} = -(\Gamma_{j,j+1} + \Gamma_{j,j-1})P(j,t) + \Gamma_{j+1,j}P(j+1,t) + \Gamma_{j-1,j}P(j-1,t)\,, \tag{1}$$

where $P(j,t)$ is the probability of finding the particle at site j at time t. The transition rates are given functions of the intersite distance, $\Gamma_{j,j+1} = \Gamma(l_j)$, and are symmetric, *i.e.* $\Gamma_{j,j+1} = \Gamma_{j+1,j}$. We consider here the particular forms of $\Gamma(l_j)$ and $\mu(l_j)$ relevant to the triplet excitations transport in disordered one-dimensional (1D) arrays of donor centers or spectrum of low-lying excitations in disordered 1D Heisenberg chain [2]. For this physical situation the probability distribution $\mu(l_j)$ has a negative exponential form

$$\mu(l_j) = n\exp(-nl_j)\,, \tag{2}$$

where n denotes the mean concentration of lattice sites; and the transition rates are exponentially decreasing functions of the intersite distance

$$\Gamma(l_j) = r\exp\left(-\frac{l_j}{a}\right)\,, \tag{3}$$

where r is the amplitude of the transfer and a is the overlapping parameter.

Let us note that the model under consideration belongs to the well-studied area of random walk in presence of random quenched barriers [1–5]. Analytical results describing the mean-square displacement (MSD) and the average propagator of a particle on such a chain were derived[1] in [1, 2] in terms of certain mean-field approach. It was shown that the single parameter which controls the behavior of the characteristics is the value $\nu = an$. In particular, it was found that the MSD grows with time in proportion to $t^{2\nu/(2+\nu)}$. However, the analysis presented in [1, 2] is quite involved and does not concern the underlying physical mechanism of the anomalous dynamics. In this section we examine behavior of the MSD, passage times and the disorder average probability current (DAPC) for this model of transport in random media using simple analysis of the representative realizations of disorder, which support anomalous behavior of these characteristics. On the basis of this analysis we recover the result for the MSD [1, 2] and obtain several new ones. Besides, we calculate rigorously the distribution function of the probability current.

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[1] This model represents the case C in the notations of [2].

2.2. Trajectories, passage times and mean square displacement

We begin with the calculation of passage times and the MSD. Consider some finite segment of the chain, which contains $N+1$ sites, $N \gg 1$. Since all the intersite distances are independent random variables, the probability of having the maximal intersite distance on this segment exactly equal to $l_{\max}$ can be written down as

$$\Pi(l_{\max}) = F^{N-1}(l_{\max})\mu^N(l = l_{\max}); \quad F(l_{\max}) = \int_0^{l_{\max}} dX\, \mu(X)\,.$$

The maximal intersite distance $l_{\max}$ is obviously greater than the mean intersite distance $\bar{l} \propto 1/n$ and we thus have in the large-N limit

$$\Pi(l_{\max}) \propto \exp(-[1 - F(l_{\max})]N)\mu(l = l_{\max})\,.$$

The maximum of $\Pi(l_{\max})$ is approached when $\Pi(l_{\max})N \propto 1$, *i.e.* $l_{\max}$ is the typical largest value of the intersite distances for which the expectation of the number of intervals is of order 1. The typical maximal intersite distance $l_{\max}$ can be estimated from the latter relation and we find that it grows with the number of sites N in the segment as $l_{\max} \propto (\log(N)/n)$. Correspondingly, the typical time needed to jump over the interval $l_{\max}$ is then estimated as

$$t_{\rm typ}(l_{\max}) \propto \frac{1}{r} N^{1/\nu}\,. \tag{4}$$

Since we have fixed $l_{\max}$ by its typical maximum value, all other distances are less than this typical value and, therefore, all other jump times have bounded distributions with finite moments of arbitrary order. In particular, if $\nu > 1$, the mean jump rate equals

$$\langle t(l, l < l_{\max})\rangle = \frac{\int_0^{l_{\max}} \exp\left(\frac{(1-\nu)\xi}{a}\right) d\xi}{r \int_0^{l_{\max}} \exp(-n\xi) d\xi} = \frac{1}{r}\frac{\nu}{\nu - 1}\,,$$

whereas if $\nu < 1$

$$\langle t(l, l < l_{\max})\rangle = \frac{1}{r}\frac{\nu}{\nu - 1} N^{1/\nu - 1}\,.$$

The sum of N independent jump times for these typical intervals is equal to $\frac{1}{r}\frac{\nu}{1-\nu} N^{1/\nu}$, *i.e.* is smaller than the right-hand-side of Eq. (4) due to the smaller value of the prefactor. Therefore, we can formulate the following statement. For $\nu < 1/2$, the particle, confined between two typical maximum intervals $l_{\max,1}$ and $l_{\max,2}$, such that $l_{\max,1} > l_{\max,2}$ and both are greater than all the inbetween intervals, has the smaller probability to cross the largest interval starting from its boundary then the probability of jumping through all the inbetween intervals until the next maximum.

Correspondingly, the most probable trajectory is organized as follows. A particle being at site j jumps through the smallest of the two neighboring intervals. It moves in the same direction until it meets the interval which is greater then the first one. Then it changes the direction and jumps until it encounters the interval which is greater than all explored before. Then it again changes the direction and the process repeats. Let us also illustrate this statement for a particular realization. Suppose a segment of the chain, containes seven sites. The intersite distance between the first and the second is l_1, the distance between the second and the third is l_2, and *etc.* Suppose next that these intervals satisfy the inequality,

$$l_6 > l_1 > l_5 > l_3 > l_4 > l_2 \,,$$

and the particle is initially located at position $j = 4$ having neighboring intervals l_3 and l_4. Then the most probable path for the first 13 steps is as follows (Fig. 1): Since $l_3 > l_4$ the particle jumps through the smallest of these two intervals, $4 \to 5$. Being at site $j = 5$ it changes its direction since $l_5 > l_3$ and jumps $5 \to 4 \to 3 \to 2$. Further on, since $l_1 > l_5$ it jumps $2 \to 3 \to 4 \to 5 \to 6$. Next, since $l_6 > l_1$ it again changes the direction and jumps $6 \to 5 \to \ldots \to 1$.

Since the particle jumps through the largest interval only from the neighboring site and the probability of finding it on each site between two maximum intervals is of the same order, the time which the particle spends on the chain segment containing N sites is proportional to the product $N t_{\rm typ}(l_{\max})$. This yields the following scaling relation between the typical displacement and time,

$$t \propto N^{1+1/\nu} \propto [\sqrt{\langle X^2(t)\rangle}]^{1+1/\nu} \tag{5}$$

and, thus, we obtain the following result for the mean square displacement

$$\langle X^2(t)\rangle \propto t^{2\nu/1+\nu} \tag{6}$$

which was first derived in [1, 2] by means of a mean-field approach.

2.3. Steady state probability current

Let us next examine the behavior of the steady state disorder average probability current J. Consider again a segment of the chain containing $N+1$ sites with fixed values of the probabilities of finding the particle at the endpoints, $P(j=0, t=\infty) = P_0$ and $P(j=N+1, t=\infty) = P_{N+1}$. From the master equation (1) one can readily find the explicit expression for the $J(N)$ for a given realization of disorder. It is defined by the recursion scheme (see, *e.g.*, Ref. [3], p.392), which in our case of the symmetric transition rates reduce to the particularly simple relations

$$P(j, t=\infty) = \frac{J(N)}{\Gamma(l_j)} + P(j+1, t=\infty).$$

Solving these equations one gets for a given realization of disorder

$$J(N) = \frac{\Delta P}{\tau(N)}, \tag{7}$$

where $\Delta P = P_0 - P_{N+1}$ and $\tau(N)$ is defined by the transparent "inverse resistivity" form

$$\tau(N) = \sum_{k=0}^{N} \frac{1}{\Gamma(l_k)}. \tag{8}$$

The disorder average probability current defined by Eqs (7), (8) can be calculated exactly. Moreover, it is possible to find all the moments of the current and the distribution function. We begin with a simple estimate of its behavior and then present more rigorous results.

Assuming that disorder average current is controlled by the largest interval between donors, we can estimate the DAPC as

$$\langle J(N) \rangle \propto \Delta P \int_N^\infty \mu(l_{\mathrm{max}}) \Gamma(l_{\mathrm{max}}) dl_{\mathrm{max}}.$$

Performing the integration, we evaluate the following dependence of the average probability current on the number of sites $N+1$ (the dependence on the sample's size is obtained trivially by substitution of $N = X/n$),

$$\langle J(N) \rangle \propto \frac{\Delta P}{N^{1/\nu}}. \tag{9}$$

Let us examine the behavior of $\tau(N)$ in Eq. (8). Using Eqs (3), (4) one can find the distribution function of variable $1/\Gamma(l_j)$. It reads

$$P\left(\tau_i = \frac{1}{\Gamma(l_j)}\right) = \nu r^{-\nu} \tau_j^{-1-\nu}, \quad \frac{1}{r} < \tau_j < \infty. \tag{10}$$

Therefore, $\tau(N)$ is the sum of N independent identically distributed random variables having a broad distribution with infinite moments. A generalized form of the central limit theorem insures that the suitably rescaled variable,

$$T(N) = \frac{\tau(N)}{N^{1/\nu}}, \quad \text{for} \quad 0 < \nu < 1,$$

or

$$T(N) = \frac{\tau(N) - N\langle\tau(N)\rangle}{N^{1/\nu}}, \quad \text{for} \quad 1 < \nu < 2;$$

$$T(N) = \frac{\tau(N) - N\langle\tau(N)\rangle}{N^{1/2}}, \quad \text{for} \quad \nu > 2;$$

and in the marginal cases

$$T(N) = \frac{\tau(N)}{N\log(N)}, \quad \text{for} \quad \nu = 1,$$

$$T(N) = \frac{\tau(N) - N\langle\tau(N)\rangle}{(N\log(N))^{1/2}}, \quad \text{for} \quad \nu = 2,$$

possesses a limit distribution $P(T(N))$ when N goes to infinity, $P(T(N)) = L_\nu(T)$, where L_ν is non-Gaussian stable (Levy) law. The explicit expressions of the stable laws are known only in two particular cases (except the trivial case $\nu > 2$, when $P(T(N))$ is the normal law). For $\nu = 1/2$, when it describes the limit distribution of the first return times of a one-dimensional Brownian motion, and for $\nu = 1/3$. However, the large-T and small-T asymptotic forms of $L_\nu(T)$ are established (see, *e.g.*, the Appendix in [6]) for any value of the parameter ν. Besides, the negative moments of $L_\nu(T)$ can be calculated exactly,

$$\int_0^\infty T^{-m} dT L_\nu(T) = Z^{-m/\nu} \frac{\Gamma(m/\nu)}{\nu\Gamma(m)}, \quad Z = \frac{\pi}{\sin(\pi\nu)\Gamma(\nu)r^\nu}.$$

Let us note that the desired average current and its moments are essentially the negative moments of the distribution $L_\nu(T)$. After some transformations we obtain the exact expression for the current moments of an arbitrary order m, if $\nu < 1$

$$\langle J^m(N)\rangle = \frac{\Gamma(m/\nu)[\Delta P]^m}{\nu\Gamma(m)(ZN)^{m/\nu}}. \tag{11}$$

Eq. (11) with $m = 1$ confirms our estimate in Eq. (9).

The knowledge of the moments in Eq. (11) or the distribution function of $\tau(N)$ suffices to evaluate the distribution function of the probability current. The latter can be readily computed from Eq. (11)

$$P(J) = (J^2 N^{1/\nu})^{-1} L_\nu \left(\frac{1}{JN^{1/\nu}}\right). \tag{12}$$

One can evaluate explicitly its asymptotic forms. For $JN^{1/\nu} \gg 1$ the normalized distribution function has a stretched-exponential form,

$$P(J) \propto \left[2\pi(1-\nu)\left(\frac{J^{2-3\nu}}{\nu ZN}\right)^{1/(1-\nu)}\right]^{-1/2} \exp\left[-\frac{1-\nu}{\nu}(\nu ZNJ^{\nu})^{1/(1-\nu)}\right]. \tag{13}$$

Within the opposite limit $N^{1/\nu}J \ll 1$ the distribution function diverges as

$$P(J) \propto \frac{ZN\Gamma(1+\nu)\sin(\pi\nu)}{\pi} J^{\nu-1}. \tag{14}$$

3. Transmission probability for a random telegraph process in a random potential

3.1. The model

We consider a particle moving on a segment $0 \le x \le L$ which has two possible velocities $\pm v$, in a presence of a potential $V(x)$. When the particle is at point x with velocity $+v$ (resp. $-v$) we shall call $a_+(x)dt$ (resp. $a_-(x)dt$) the probability that in the time interval $(t, t+dt)$ the particle changes its velocity from $+v$ to $-v$ (resp. from $-v$ to $+v$) due to the collisions with an external bath. Let us also denote by $P_\pm(x,t)dx$ the probability that the particle is in the interval $x, x+dx$ with velocity $\pm v$ at time t.

It is easy to see that $P_\pm(x,t)$ satisfy the following system

$$\frac{\partial P_\alpha}{\partial t} = -\nu\frac{\partial P_\alpha}{\partial x} - (a_\alpha P_\alpha - a_{-\alpha}P_{-\alpha}), \tag{15}$$

with $a = +$ or $-$. Here a should be such that the thermal equilibrium distribution in potential V is a stationary solution of (15), namely we impose that $P_+ = P_- = e^{-\beta V}$ is a solution of (15). This implies

$$a_+ - a_- = v\beta\frac{dV}{dx}. \tag{16}$$

3.2. Transmission flux

We want to compute the transmission flux for this stochastic process. This is

$$\Phi_L = vS_L,$$

where S_L is the probability that a particle which is released at 0 with velocity $+v$, is transmitted at L (*i.e.*, gets out from the interval $[0, L]$ through L). We have

$$S_L = \left(1 + \int_0^L \exp[\beta(V(x)V(0))] \frac{a_+(x)dx}{v}\right)^{-1} . \qquad (17)$$

One direct method to see this result is the following: we discretize the interval $[0, L]$ in small intervals

$$\left[\frac{iL}{N}, \frac{(i+1)L}{N}\right] \quad \text{for} \quad 0 \le i \le N-1$$

and we call $S_{i,i+1}$ the probability to be absorbed by $i+1$ starting from i with positive velocity, and $S_{i+1,i}$ the probability to be absorbed by i, starting from $i+1$ with negative velocity. We also define q_i by the detailed balance conditions

$$q_i S_{i,i+1} = q_{i+1} S_{i+1,i} .$$

It is clear that

$$S_{i,i+1} = 1 - a_+ \frac{dx}{v} ,$$
$$S_{i+1,i} = 1 - a_- \frac{dx}{v} ,$$

$(dx = L/N)$, so that

$$\frac{q_i}{q_{i+1}} = 1 - \frac{a_- - a_+}{v} dx = 1 - \beta V' dx$$

(due to relation (17)) and q_i is proportional to $e^{-\beta V}$ as we already know. Moreover, it is well known (under much more general circumstances, see [6]) that

$$\frac{1}{q_0}\left(\frac{1}{S_L} - 1\right) = \sum_{k=0}^{N-1} \frac{1}{q_k}\left(\frac{1}{S_{k,k+1}} - 1\right) ,$$

so that

$$e^{\beta V(0)}\left(\frac{1}{S_L} - 1\right) = \int_0^L \exp(\beta V) \frac{a_+(x)dx}{v}$$

which is (17).

3.3. Normal transmission probability

We shall now assume that V is a random potential with the following structure : the interval $[0, L]$ is divided into N intervals of length $\varepsilon = L/N$. In the interval $(i\varepsilon, (i+1)\varepsilon)$, we assume that the potential V takes a constant value V_i with the following rules:

(i) $V_0 = 0$

(ii) V_i are independent identically distributed random variables W such that

$$\mathrm{Prob}(W = w_k) = p_k\,, \tag{18}$$

where w_k are given values and $\sum_{k=1}^{\infty} p_k = 1$. We also assume that a_+ is constant.

We want to compute the average value $\langle S_L \rangle$. Let us call

$$K = \frac{a_+}{v}\,,$$

then it is easy to see that

$$< S_L > = \int_0^{\infty} \mathrm{e}^{-\theta} \left\langle \exp\left(-\theta K \int_0^L \mathrm{e}^{\beta V} dx \right) \right\rangle d\theta$$

$$= \int_0^{\infty} \mathrm{e}^{-\theta} \left\langle \exp\left(-\theta K \varepsilon \mathrm{e}^{\beta W} \right) \right\rangle^N d\theta\,.$$

Let us change the variables and write $xi = \mathrm{e}^{-\theta K \varepsilon}$. The previous formula becomes

$$\langle S_L \rangle = \frac{1}{K\varepsilon} \int_0^1 \xi^{\frac{1}{K\varepsilon}-1} \exp\left(\frac{L}{\varepsilon} \varphi(\xi) \right) d\xi\,, \tag{19}$$

where we have defined:

$$\varphi(\xi) = \log\left(\sum_{k=1}^{\infty} p_k \xi^{\exp(\beta w_k)} \right). \tag{20}$$

The function $\varphi(\xi)$ increases over the interval [0,1] and takes its maximum 0 at point $\xi = 1$. When ε is fixed, but L tends to infinity, we see from formula (20) that the maximal contribution to the integral is obtained at $\xi = 1$ so that

$$\langle S_L \rangle \sim \frac{1}{K\varepsilon} \left(\frac{L}{\varepsilon} \frac{d}{d\xi} \varphi(\xi)|_{\xi=1} \right)^{-1}, \tag{21}$$

provided that

$$\frac{d}{d\xi}\varphi(\xi)|_{\xi=1} < +\infty\,. \tag{22}$$

With hypothesis (21) we obtain

$$\langle S_L\rangle \sim \frac{1}{L}\left(K\left(\sum_{k=1}^{\infty} p_k \xi^{\exp(\beta w_k)}\right)\right)^{-1} \tag{23}$$

or

$$\langle S_L\rangle \sim \left(\int_0^L \frac{a_+}{v}\left\langle e^{\beta W}\right\rangle dx\right)^{-1}\,. \tag{24}$$

In other words the average of the inverse quantity $\int_0^L e^{\beta W}$ is the inverse of the average and we obtain a normal flux in L^{-1}.

3.4. Abnormal subdiffusive flux

Let us now assume that

$$\left.\frac{d}{d\xi}\varphi(\xi)\right|_{\xi=1} = +\infty \tag{25}$$

which means that

$$\langle e^{\beta W}\rangle \equiv \sum_{k=1}^{\infty} p_k \exp(\beta w_k) = +\infty\,. \tag{26}$$

In this case, (20) is still valid, but the evaluation (22) does not hold any more. Under hypothesis (25), $\varphi(\xi)$ is still increasing on [0,1], and continuous at $\xi = 1$, but it is not differentiable at $\xi = 1$. Let us assume that $\varphi(\xi)$ satisfies a Hölder condition for some $0 \le \gamma < 1$

$$\varphi(\xi) \sim -A|\xi - 1|^{\gamma}\,. \tag{27}$$

Define a new variable η by

$$\eta = \frac{AL}{\varepsilon}|\xi - 1|^{\gamma}\,. \tag{28}$$

It is easy to see that, when L tends to infinity

$$\langle S_L\rangle \sim \frac{C}{L^{1/\gamma}}\,, \tag{29}$$

where C is some constant, so that the transmission probability presents a subdiffusive behavior.

For example, let us assume that the values w_k of W are thermally distributed with another temperature β'^{-1} different from β, so that

$$p_k \sim e^{-\beta w_k} .$$

In this case, if we denote $\alpha_k = \exp(\beta w_k)$, we have

$$\varphi(\xi) = \log \left(\sum_{k \geq 1} \alpha_k^{-\beta/\beta} \xi^{\alpha_k} \right) . \tag{30}$$

Let us further assume that the series inside the logarithm is a lacunary series, namely that

$$\frac{\alpha_{k+1}}{\alpha_k} \geq 1 + \varepsilon ,$$

for some fixed ε. Then if $\frac{\beta'}{\beta} > 1$, φ is differentiable at $\xi = 1$ and we have a normal flux of the type (23), $\langle S_L \rangle \sim L^{-1}$.

If, however, $\frac{\beta'}{\beta} < 1$, it is a consequence of the theory of lacunary Fourier series that

$$\sum \alpha_k^{-\beta/\beta} \xi^{\alpha_k}$$

is Hölder continuous at $\xi = 1$ with an exponent $\gamma = \frac{\beta'}{\beta}$ (see for example [7]) so that if $\beta'/\beta < 1$, we have a reduced flux $\langle S_L \rangle \sim L^{-\beta'/\beta}$. The case $\beta' = \beta$ is slightly more complicate and gives the behavior $\langle S_L \rangle \sim (L \log L)^{-1}$.

It is seen that these conclusions are exactly similar to those of Section 2, where the parameter $\nu = an$ plays the role of β'/β in the present section.

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