Variable range random walk

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Abstract
Exploiting the coherent medium approximation, random walk among sites distributed randomly in space is investigated when the jump rate depends on the distance between two adjacent sites. In one dimension, it is shown that when the jump rate decays exponentially in the long distance limit, a non-diffusive to diffusive transition occurs as the density of sites is increased. In three dimensions, the transition exists when the jump rate has a super Gaussian decay.

1 Introduction
Random walk is highly robust which has been applied in almost all areas of science including biology, materials sciences, economics and social phenomena [1]. It has also been exploited in the description of structural evolution by the free energy landscape theory of non-equilibrium systems [2]. Random walk is generally formulated on lattices and complex networks [3]. In some applications, a random walker is assumed to make jumps among sites randomly distributed in space [4]. In Mott’s variable range hopping model [5], carriers are allowed to make a long range hopping in disordered media. Diffusion processes have also been investigated when the diffusivity depends on position and time [6].
In this paper, I investigate a random walk among randomly distributed sites, where a walker makes a jump from a site to its adjacent neighbor on a limited solid angle along a fixed number of directions. The jump rate is assumed to depend on the distance between two sites. Since sites are distributed randomly, the walker makes jumps with variable ranges. I obtain the diffusion constant within the coherent medium approximation \[7\] and discuss the possibility of a transition from non-diffusive to diffusive states.

In §2, I explain the model in some detail and the method of analysis based on the coherent medium approximation. In §3, I study the random walk in one dimension for three different types of the jump rate and discuss non-diffusive to diffusive transition for an extended percolation model. The random walk in three dimensions is investigated in §4 and results are discussed in §5,

## 2 Model and the method of analysis

I consider a random walk, where the transition probability of the random walker obeys

$$\frac{\partial P(r_n, t|r_0, 0)}{\partial t} = - \sum_m w(|r_m - r_n|) P(r_n, t|r_0, 0) + \sum_m w(|r_n - r_m|) P(r_m, t|r_0, 0). \quad (1)$$

Here, $P(r_n, t|r_0, 0)$ denotes the transition probability that a random walker is at the site $r_n$ at time $t$ when it started $r_0$ at time $t = 0$, and $w(|r_m - r_n|)$ is the jump rate of a random walker from site $r_n$ to site $r_m$. I assume that $w(|r_m - r_n|)$ is a function of the distance between $r_n$ and $r_m$. Usually, $w(r)$ is assumed to be nonzero within a certain distance. For example, the percolation process on lattices is modeled by jumps of a random walker within nearest neighbor sites. In this paper, I introduce an extended percolation model in which a random walker can make a longer jump with smaller rate beyond the limited distance used for the standard percolation model.
The diffusion constant $D$ is given by

$$D = \lim_{u \to 0} \frac{u^2}{2d} \sum_m \langle (\mathbf{r}_m - \mathbf{r}_0)^2 \tilde{P}(\mathbf{r}_m, u|\mathbf{r}_0) \rangle,$$  \hspace{1cm} (2)

where

$$\tilde{P}(\mathbf{r}_m, u|\mathbf{r}_0) = \int_0^\infty P(\mathbf{r}_m, t|\mathbf{r}_0, 0)e^{-ut}dt$$ \hspace{1cm} (3)

is the Laplace transform of the transition probability $P(\mathbf{r}_m, t|\mathbf{r}_0, 0)$, $d$ is the dimension of the space and $\langle \cdot \cdot \cdot \rangle$ denotes an ensemble average over the random distribution of sites. I exploit the coherent medium approximation for positionally disordered systems \cite{7,8}. I first divide the space around a site into $z$ equivalent cones and assume that a random walker makes a jump to the adjacent site in one of the $z$ cones. Within this approximation, the normalized diffusion constant is given by

$$\frac{D}{D_0} = \frac{w_c}{w_0},$$ \hspace{1cm} (4)

where $D_0$ and $w_0$ are the diffusion constant and jump rate of a reference regular system and $w_c$ is the coherent jump rate which is determined self-consistently by

$$2zw_c = \int_0^\infty \frac{N(r)dr}{(\frac{z}{2} - 1)w_c + w(r)}.$$ \hspace{1cm} (5)

Here $N(r)$ represents the distribution function of the distance between adjacent neighbors in a cone. In three dimensions,

$$N(r) = \frac{4\pi r^2n}{z} \exp \left(-\frac{4\pi r^2n}{3z}\right)$$ \hspace{1cm} (6)

when sites are distributed randomly with density $n$. In Eq. (4), the scale of the length of the system under consideration is assumed to be the same as that of the reference system since it does not play any significant role here.
3 Extended percolation in one dimension

In one dimension, \( z \) is set to \( z = 2 \) in Eq. (5) and the self-consistency equation for the coherent jump rate \( w_c \) reads as

\[
\frac{1}{w_c} = \int_0^\infty N(x) \frac{dx}{w(x)},
\]

and the distribution function \( N(x) \) becomes

\[
N(x) = ne^{-nx}.
\]

In this section, I investigate several different forms of \( w(x) \) which is considered as a percolation model with long range connection, and discuss possibility of a diffusive to non-diffusive transition.

3.1 Simple percolation model

As the simplest model, I first consider a transition probability

\[
w(x) = \begin{cases} w_0 & \text{(when } 0 \leq x \leq r_0) \\ \epsilon w_0 & \text{(when } x > r_0 \text{ and } \epsilon \to 0) \end{cases}.
\]

It is straightforward to obtain the diffusion constant from Eqs. (4) and (7) \(~(9)\). I find

\[
\frac{D}{D_0} = \frac{1}{1 + \frac{1}{\epsilon} e^{-nx_0}},
\]

and Fig. 1 shows the dependence of \( D/D_0 \) on the scaled density \( nx_0 \) for \( \epsilon = 10^{-2}, 10^{-3}, 10^{-4} \).

As expected, the diffusion constant is identically zero in the percolation limit \( \epsilon = 0 \). When \( \epsilon \) is finite, the diffusion constant is given by a sigmoid function whose inflection point is at \( nx_0 = -\ln[\epsilon/(1 - \epsilon)] \).

3.2 Extended percolation model

I define an extended percolation model by a jump rate

\[
w(x) = \begin{cases} w_0 & \text{(when } 0 \leq x \leq x_0) \\ w_0 \left( \frac{x_0}{x} \right)^\alpha & \text{(when } x > x_0) \end{cases},
\]

\[
(11)
\]
Figure 1: The scaled diffusion constants of a simple percolation model Eq. (9) are shown as functions of the scaled density for $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$.

where $\alpha > 0$ is assumed. Namely, in this model, the range of jump beyond $x_0$ decays as a power-law function with exponent $-\alpha$. From Eqs. (4), (7), (8) and (11), I find

$$\frac{D}{D_0} = 1 - e^{-nx_0} + \left(\frac{nx_0}{e^{nx_0}} - 1\right)\Gamma(\alpha + 1, nx_0),$$

where $\Gamma(s, x) \equiv \int_x^\infty e^{-t}t^{s-1}dt$ is the upper incomplete Gamma function. Figure 2 shows the $nx_0$ dependence of the diffusion constant for $\alpha = 1, 5, 10, 20$.

The diffusion constant becomes identically zero at $\alpha = \infty$, since $\alpha = \infty$ corresponds to the percolation limit.

### 3.3 Logistic-type model

I consider a smooth function for the jump rate represented by a kind of the logistic curve

$$w(x) = w_0 \frac{e^{x_+ / x_0} - 1}{e^{x_+ / x_0} + e^{x / x_0} - 2},$$

which satisfies $w(0) = w_0, w(x_+) = w_0/2$ and $w(\infty) = 0$. The diffusion constant is given by

$$\frac{D}{D_0} = 1 - \frac{1}{1 + (e^{-x_+ / x_0} - 1)(nx_0 - 1)},$$

$5$
Figure 2: Scaled diffusion constants for an extended percolation model Eq. (11) are shown as functions of the scaled density for $\alpha = 1, 5, 10, 20$.

Figure 3 shows the diffusion constant as functions of $n x_0$ for $x_r/x_0 = 1.1, 2, 3$. Consequently, there is a non-diffusive to diffusive transition at $n x_0 = 1$. Since $D/D_0 \simeq (e^{-x_r/x_0} - 1)(n x_0 - 1)$ when $n x_0 \sim 1$, the critical exponent of the diffusion constant is unity.

Figure 3: Scaled diffusion constants for a logistic-type model Eq. (13) are shown as functions of the scaled density for $x_r/x_0 = 1.1, 2, 3$. 

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4 Extended percolation in three dimensions

4.1 Extended percolation model

I consider an extended percolation model in three dimensions where sites are distributed randomly with density $n$ in a three dimensional space and the jump rate $w(r)$ is given by

$$w(r) = \begin{cases} 
  w_0 & \text{(when } 0 \leq r \leq r_0) \\
  w_0 \left( \frac{r}{r_0} \right)^\alpha & \text{(when } r > r_0) 
\end{cases}$$

(15)

Self-consistency equations (5) and (6) for $w_c$ with Eq. (15) are solved numerically. Figure 4 shows the dependence of the scaled diffusion constant $D/D_0$ on the scaled density $(4\pi r_0^2/3)n$ for $\alpha = 10$ and $\infty$, where $z = 6$ is used as an example. There are no percolation transition for $\alpha < \infty$. The case $\alpha = \infty$ is the simple percolation model, the diffusion constant of which is given by

$$\frac{D}{D_0} = 1 - \frac{z}{z-2} \exp \left( -\frac{4\pi r_0^2}{3z} n \right)$$

(16)

and the critical percolation density is given by

$$\left( \frac{4\pi r_0^2}{3} n \right)_c = z \ln \frac{z}{z-2}$$

(17)

When $z = 6$, $\left( \frac{4\pi r_0^2}{3} n \right)_c = 2.43$. 

![Figure 4: The dependence of the scaled diffusion constant on the scaled density for the extended percolation model for $\alpha = 10, \infty$. Note $\alpha = \infty$ corresponds to the standard percolation model.](image-url)
4.2 Super exponential decay model

I consider the jump rate $w(r)$ given by

$$w(r) = \begin{cases} w_0 & \text{(when } 0 \leq r \leq r_0) \\ w_0 \exp\{-[k(r - r_0)]^{\beta}\} & \text{(when } r > r_0) \end{cases}$$

(18)

Figure 5 represents the dependence of the scaled diffusion constant $D/D_0$ on the scaled density $(4\pi r_0^3/3)n$ for $\beta = 1, 4$, where $kr_0 = 3$ and $z = 6$ are used. Apparently, there is a non-diffusive to diffusive transition for $\beta = 4$. In fact, a non-diffusive to diffusive transition exists when $\beta \geq 3$.

5 Discussion

I have studied random walks where a random walker can make long range jumps and obtained characteristic behavior of the diffusion constant within the coherent medium approximation. As for the distance dependence of the jump rate, I investigated different types of extended percolation models. It is shown that a non-diffusive to diffusive transition exists in certain types of the jump rate function in one and three dimensions.
The self-consistency Eq. \(5\) supports a solution \(w_c = 0\) only when
\[
\int_0^\infty \frac{N(r)dr}{w(r)} = \infty. \tag{19}
\]
Therefore, in one dimension, the non-diffusive to diffusive transition exists when the jump rate function exhibits exponential or faster decay in the long distance limit \([8]\). In \(d\)-dimensional systems, there are no non-diffusive states unless the jump rate function decays faster than \(e^{-r^d}\).

The present results will give some insights in random walks in a highly complex structure like the free energy landscape.

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