ONE-DIMENSIONAL HOPPING TRANSPORT IN ENERGETICALLY DISORDERED SYSTEMS IN PRESENCE OF A STRONG BIASED FIELD

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This report is devoted to the study of hopping drift mobility of charge carries in one-dimensional regular chain of localization site with energetic disorder. The individual jump rate was assumed to follow Miller-Abrahams type transition with nearest neighbor hopping. Exact results were obtained for the temperature and field dependence of the diffusion constant $D(T, E)$ and drift velocity $V(T, E)$ in a system with uncorrelated energetic disorder.

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1. INTRODUCTION

The hopping drift motion in a one-dimensional regular chain of localization sites with energetic disorder has been studied extensively as a simple model for carrier or excitation transport in disordered systems. This model gives a satisfactory understanding of conductivity experiments on many disordered organic solids, such as molecularly doped polymers, conjugated polymers and deoxyribonucleic acids [1]. In calculation of hopping mobility the important quantity is the elementary jump rate from site i to j with the energy difference Δ. In the case of low temperatures the jump rate can be represented in the form suggested by Miller and Abrahams:

$$\Gamma_{i,j} = \Gamma_0 \exp\left(-\frac{d_{ij}}{a}\right) f\left(\Delta_{i,j}\right), \qquad (1)$$

where d_{ij} is the distance between the sites, a is the localization length. The function f is related to the energy gain or energy loss during the jump,

$$f(\alpha) = \begin{cases} 1, & \text{if } \alpha \geq 0; \\ e^{\alpha/T}, & \text{if } x < 0. \end{cases}$$

In the limit of low concentration of charge carriers that the statistical and dynamic interaction between the carriers can be ignored, the bare energy difference between sites is $\Delta_{i,j} = \varepsilon_j - \varepsilon_i - eEr_{ij}$. Here ε_i is the random energy of localized site i, e denotes the electron charge, and r_{ij} is the projection of the vector connecting site i and j on the field direction. In one-dimensional hopping model with nearest neighbor hops the motion of carrier can be describe by the standard rate equation for occupational probability:

$$\frac{dP_i}{dt} = -\left(\Gamma_{i,i+1} + \Gamma_{i,i-1}\right) P_i$$
$$+\Gamma_{i+1,i} P_{i+1} + \Gamma_{i-1,i} P_{i-1}; \qquad (2)$$
$$P_i(0) = \delta_{i,0},$$

where at time $t = 0$ the particle is localized on site $i = 0$. The transfer rates are random variables and not symmetrical. Nearest neighbor hopping within the model described by $(1), (2)$ has been recently studied by both analytically and numerically [2, 3]. Exact results were obtained for the temperature and field dependence of the drift velocity in such system [4]. The aim of present study is to continue the analysis one-dimensional hopping model with site disorder. We give further development of the analytical theory and receive an exact expression for the diffusion constant of a one-dimensional hopping problem with uncorrelated site energy distribution. The method used is based on the approach suggested in Ref. [3]

2. THE ANALYTICAL MODEL

We are interested in a long-time asymptotic behavior of the fist two moments of the particle position $\langle x(t) \rangle$ and $\langle x^2(t) \rangle$. This problem has been extensively studied and the explicit formulation of mean velocity V_N and effective diffusion constant D_N have been obtained in [2, 3] for a periodic one-dimensional hopping model of arbitrary period N. Further we will follow the approach suggested in [3]. Then

$$V_N = \frac{N}{\sum_{i=1}^{N} G_i^{-1}}, \quad D_N = [V_N]^3 \frac{1}{N} \sum_{i=1}^{N} \frac{1 + 2g_i}{2\left[G_i\right]^2}, \qquad (3)$$

where

$$\frac{1}{G_n} = \frac{\left(\frac{1}{\Gamma_{n,n+1}}\right) + \sum_{i=n+1}^{n+N-1} \left(\frac{1}{\Gamma_{i,i+1}}\right) \prod_{j=n}^{i-1} \left(\frac{\Gamma_{j+1,j}}{\Gamma_{j,j+1}}\right)}{1 - \prod_{i=1}^{n+N-1} \left(\frac{\Gamma_{i+1,i}}{\Gamma_{i,i+1}}\right)}, \qquad (4)$$

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$$\frac{g_n}{[G_n]^2} = \frac{\sum_{i=n+1}^{n+N-1} (G_i)^{-2} \prod_{j=n}^{i-1} (\Gamma_{j+1,j}/\Gamma_{j,j+1})}{1 - \prod_{i=1}^{n+N-1} (\Gamma_{i+1,i}/\Gamma_{i,i+1})}. \tag{5}$$

In accordance with Eq. (1), the ratio of forward $\Gamma_{i,i+1}$ and backward $\Gamma_{i+1,i}$ hopping rates for any pair of neighboring sites is

$$\frac{\Gamma_{i+1,i}}{\Gamma_{i,i+1}} = e^{-F} \frac{p_0(\varepsilon_i)}{p_0(\varepsilon_{i+1})}, \tag{6}$$

where F is the positive dimensionless energy parameter $F = eaE/T$, and $p_0(\varepsilon)$ is the equilibrium distribution function $p_0(\varepsilon) = \exp(-\varepsilon/T)$. It is supposed that the electric field $\vec{E}$ is put along the negative direction of the axis X, so that the drift velocity of negative charged carriers is occurred along X axis. According Eq. (3) the drift velocity V and diffusion coefficient D are self averaging quantities. In the limit $N \to \infty$ one obtains

$$V = \left\langle [G_i]^{-1} \right\rangle,$$

$$D = V^3 \left(\left\langle \frac{1}{2[G_i]^2} \right\rangle + \left\langle \frac{g_i}{[G_i]^2} \right\rangle \right). \tag{7}$$

If we average each member of Eq. (4) with respect to the independent random distribution of local energies $\{\varepsilon_i\}$ and substitute in [4], we get:

$$V^{-1} = \left\langle \frac{1}{\Gamma_{n,n+1}} \right\rangle + \frac{e^{-F} \langle p_0(\varepsilon_n) \rangle}{1 - e^{-F}} \left\langle \frac{1}{p_0(\varepsilon_n)\Gamma_{n,n+1}} \right\rangle. \tag{8}$$

The calculation of diffusion coefficient D is more complicated task, because of correlations between neighboring rates Γ. Averaging Eq. (5), we have

$$\left\langle \frac{g_n}{[G_n]^2} \right\rangle = \frac{e^{-F} \langle p_0(\varepsilon_n) \rangle}{1 - e^{-F}} \left\langle \frac{1}{p_0(\varepsilon_{n+1})[G_{n+1}]^2} \right\rangle. \tag{9}$$

It is useful to represent the Eq. (4) in form of recurrent relation. From Eqs. (4) and (6) we get

$$\frac{1}{G_n} = \frac{1}{\Gamma_{n,n+1}} + e^{-F} \frac{p_0(\varepsilon_n)}{p_0(\varepsilon_{n+1})} \frac{1}{G_{n+1}}. \tag{10}$$

By squaring this relation and using the average for each member we obtain:

$$\left\langle \frac{1}{(G_n)^2} \right\rangle = \left\langle \frac{1}{(\Gamma_{n,n+1})^2} \right\rangle + \left\langle \frac{p_0(\varepsilon_n)}{\Gamma_{n,n+1}} \frac{2e^{-F}}{p_0(\varepsilon_{n+1})G_{n+1}} \right\rangle + \left\langle (p_0(\varepsilon_n))^2 \right\rangle \left\langle \frac{e^{-2F}}{(p_0(\varepsilon_{n+1})G_{n+1})^2} \right\rangle, \tag{11}$$

$$\left\langle \frac{1}{(p_0(\varepsilon_n)G_n)^2} \right\rangle = \left\langle \frac{1}{(p_0(\varepsilon_n)\Gamma_{n,n+1})^2} \right\rangle + \left\langle \frac{2e^{-2F}}{(p_0(\varepsilon_n)\Gamma_{n,n+1})(p_0(\varepsilon_{n+1})G_{n+1})} \right\rangle + \left\langle \frac{e^{-2F}}{(p_0(\varepsilon_{n+1})G_{n+1})^2} \right\rangle, \tag{12}$$

$$\left\langle \frac{1}{p_0(\varepsilon_n)(G_n)^2} \right\rangle = \left\langle \frac{1}{p_0(\varepsilon_n)(\Gamma_{n,n+1})^2} \right\rangle + \left\langle \frac{2e^{-F}}{\Gamma_{n,n+1}p_0(\varepsilon_{n+1})G_{n+1}} \right\rangle + \langle p_0(\varepsilon_n) \rangle \left\langle \frac{e^{-2F}}{(p_0(\varepsilon_{n+1})G_{n+1})^2} \right\rangle. \tag{13}$$

The same computations can be performed to additional unknown terms in (11), (12) and (13) and give:

$$\left\langle \frac{1}{(G_n)^2} \right\rangle = \left\langle \frac{1}{(\Gamma_{n,n+1})^2} \right\rangle + 2 \left(\frac{e^{-2F}}{1 - e^{-F}} \right) \left(\frac{e^{-2F}}{1 - e^{-2F}} \right) (p_0(\varepsilon_n))^2 \left\langle \frac{1}{p_0(\varepsilon_n)\Gamma_{n,n+1}} \right\rangle \left\langle \frac{1}{p_0(\varepsilon_{n+1})\Gamma_{n+1,n+2}} \right\rangle +$$

$$+ 2e^{-F} \left\{ \left\langle \frac{p_0(\varepsilon_n)}{p_0(\varepsilon_{n+1})\Gamma_{n,n+1}\Gamma_{n+1,n+2}} \right\rangle + \left(\frac{e^{-F}}{1 - e^{-F}} \right) \left\langle \frac{p_0(\varepsilon_n)}{\Gamma_{n,n+1}} \right\rangle \left\langle \frac{1}{p_0(\varepsilon_{n+1})\Gamma_{n+1,n+2}} \right\rangle \right\} + \tag{14}$$

$$+ \left(\frac{e^{-2F}}{1 - e^{-2F}} \right) \left\langle (p_0(\varepsilon_n))^2 \right\rangle \left\{ \left\langle \frac{1}{(p_0(\varepsilon_n)\Gamma_{n,n+1})^2} \right\rangle + 2e^{-F} \left\langle \frac{1}{p_0(\varepsilon_n)\Gamma_{n,n+1}} \frac{1}{p_0(\varepsilon_{n+1})\Gamma_{n+1,n+2}} \right\rangle \right\} .$$

$$\left(\frac{\langle p_0(\varepsilon_n) \rangle e^{-F}}{1 - e^{-F}} \right)^{-1} \left\langle \frac{g_n}{(G_n)^2} \right\rangle = \left\langle \frac{1}{p_0(\varepsilon_n)(\Gamma_{n,n+1})^2} \right\rangle + 2e^{-F} \left\langle \frac{1}{p_0(\varepsilon_{n+1})\Gamma_{n,n+1}\Gamma_{n+1,n+2}} \right\rangle +$$

$$+ \left(\frac{2e^{-2F}}{1 - e^{-F}} \right) \left\langle \frac{1}{\Gamma_{n,n+1}} \right\rangle \left\langle \frac{1}{p_0(\varepsilon_{n+1})\Gamma_{n+1,n+2}} \right\rangle + \left(\frac{\langle p_0(\varepsilon_n) \rangle e^{-2F}}{1 - e^{-2F}} \right) \left\langle \frac{1}{(p_0(\varepsilon_n)\Gamma_{n,n+1})^2} \right\rangle +$$

$$+ \left(\frac{2\langle p_0(\varepsilon_n) \rangle e^{-3F}}{1 - e^{-2F}} \right) \left\langle \frac{1}{p_0(\varepsilon_n)p_0(\varepsilon_{n+1})\Gamma_{n,n+1}\Gamma_{n+1,n+2}} \right\rangle + \tag{15}$$

$$+ \left(\frac{2\langle p_0(\varepsilon_n) \rangle e^{-4F}}{(1 - e^{-2F})(1 - e^{-F})} \right) \left\langle \frac{1}{p_0(\varepsilon_n)\Gamma_{n,n+1}} \right\rangle \left\langle \frac{1}{p_0(\varepsilon_{n+1})\Gamma_{n+1,n+2}} \right\rangle .$$

At low electrical fields $F \to 0$ these exact expressions can be approximated by

$$V_0 = F \left(\langle p_0(\varepsilon_n) \rangle \left\langle \frac{1}{p_0(\varepsilon_n)\Gamma_{n,n+1}} \right\rangle \right)^{-1}, \tag{16}$$

$$D_0 = \left(\langle p_0(\varepsilon_n) \rangle \left\langle \frac{1}{p_0(\varepsilon_n)\Gamma_{n,n+1}} \right\rangle \right)^{-1}. \tag{17}$$

It is obvious that these equations obey the Einstein relation at low electrical field $D_0 = FV_0$. In opposite

case of infinitely high fields (non-Ohmic regime) we have:

$$V_\infty = \left\langle (\Gamma_{n,n+1})^{-1} \right\rangle^{-1}, \qquad (18)$$
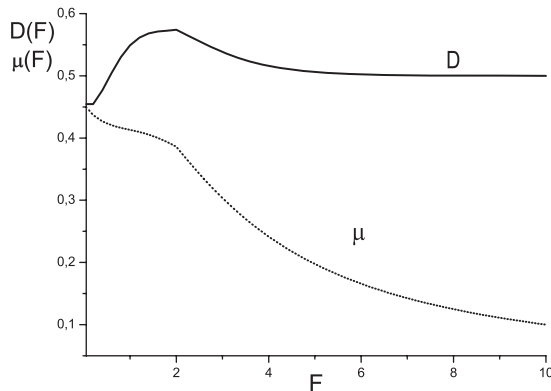
$$D_\infty = \frac{1}{2} \left\langle \frac{1}{(\Gamma_{n,n+1})^2} \right\rangle \left\langle \frac{1}{\Gamma_{n,n+1}} \right\rangle^{-3}. \qquad (19)$$

3. RESULTS

In order to study the role of the energetic disorder for the hopping transport properties we choose the simple model with a bimodal site energy distribution:

$$\psi(\varepsilon) = c\delta(\varepsilon - \varepsilon_0) + (1-c)\delta(\varepsilon) \qquad (20)$$

with $c = 0.8$ and $\varepsilon_0 = 2$ in dimensionless units.

Field dependence of the drift mobility $\mu(F)$ (the dotted line) and diffusion coefficient $D(F)$ (solid line) for the energy parameter $\varepsilon_0 = 2$, and the concentration $c = 0.8$

The results of calculations for the drift mobility $\mu = V/F$ and diffusion coefficient D according to (14) and (15) are shown in the figure.

This behavior of hopping transport accords with a number of experimental results where was observed the decrease of drift mobility with increasing electrical field. In the case of infinite electrical field we have unidirectional transport regime which can be described by means of trivial Poisson process.

4. CONCLUSIONS

We have shown that the hopping transport on bond disordered cubic lattice in presence of uniform biasing field can be described on the basis of the effective medium theory which takes into account the field-created traps. If these types of disorder are uncorrelated, the resulting drift velocity can be factorized into the random-trap and random-bond contributions. The theory is characterized by d independent parameters describing the drift velocity and diffusion coefficients for each crystal axis. It is shown that theoretical results are well consistent with a Monte Carlo simulation [4] and correctly described the occurrence of negative differential conductivity in a system with bond disorder.

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ПРЫЖКОВЫЙ ТРАНСПОРТ В ОДНОМЕРНОЙ СИСТЕМЕ С ЭНЕРГЕТИЧЕСКИМ БЕСПОРЯДКОМ В СИЛЬНОМ ВНЕШНЕМ ПОЛЕ

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Исследуется прыжковый дрейф носителей заряда в одномерной регулярной решетке с энергетическим беспорядком. Предполагается, что прыжки происходят между ближайшими узлами по закону Миллера-Абрахамса. Получены точные аналитические выражения для температурной и полевой зависимости коэффициента диффузии и скорости дрейфа для системы с не коррелированным беспорядком энергий.

СТРИБКОВИЙ ТРАНСПОРТ В ОДНОМІРНІЙ СИСТЕМІ З ЕНЕРГЕТИЧНИМ БЕЗЛАДОМ У СИЛЬНОМУ ЗОВНІШНЬОМУ ПОЛІ

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Досліджується стрибковий дрейф носіїв заряду в одномірній регулярній гратці з енергетичним безладдям. Передбачається, що стрибки відбуваються між найближчими вузлами за законом Міллера-Абрахамса. Отримані точні аналітичні вирази для температурної й польової залежності коефіцієнта дифузії й швидкості дрейфу для системи з не корельованим безладдям енергій.