THE FIELD DEPENDENCE OF THE HOPPING TRANSPORT IN BOND-DISORDERED SYSTEMS

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In this report we derive a new version of effective-medium theory for uniform biased diffusion which takes into account both field-created traps and bond disorder. The two random quantities are assumed to be independent. It is shown that theoretical results are well consistent with a Monte Carlo simulation and correctly described the occurrence of negative differential conductivity in a system with bond disorder.

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1. INTRODUCTION

The problem of drift and diffusion of carriers in energetically and spatially disordered systems in the presence of a strong biasing field is in the focus of intensive theoretical and experimental studies during several decades. One of the mostly discussed topics is whether the negative differential conductivity (NDC) is possible in such systems. The possibility of NDC for hopping transport was first discussed by Bottger and Bryksin [1]. They have developed a simple effective-medium theory for uniformly biased systems with bond disorder. This theory predicts that at not too high fields the differential hopping conductivity decreases with increasing field. The basic disadvantage of this approach is dependence of a percolation threshold for uniformly biased systems with bond disorder from an external field. It is consequence of the assumption that their effective medium theory can be characterized by a single independent parameter.

However, the recent self-consistent effective-medium theory for drift and diffusion at electrical fields [2] has not shown any decrease in the mobility with increasing field. This result does not exclude, however, the possibility of the NDC in the hopping drift. Shklovskii and co-workers suggested that NDC can be identified as arising from so-called "field-induced traps" [3]. Furthermore computer simulation of Gartstein and Conwell [4] confirmed qualitatively the existence of NDC effects in bond disorder model though no quantitative comparison with the theory has been attempted.

The goal of the present study is to develop an effective-medium theory for uniformly biased system with bond disorder which would be free of the shortcomings mentioned. Here we generalize the self-consistent theory of Parris and Bookout [2] by means of the account of "field induced traps". This makes it possible to improve the analytical results and ones of computer simulation [4].

2. BASIC EQUATIONS

We consider here the random motion of a carrier on a disordered d-dimensional cubic lattice with nearest-neighbor jumps in presence uniform biased field. The basic quantity to be calculated is the conditional probability $P_{n/m}(t)$ of finding the carrier at site $\mathbf{n}$ at time t when it was at site $\mathbf{m}$ at $t = 0$. It satisfies a master equation

$$\frac{dP_{n/m}(t)}{dt} = \sum_g \left(W_{n+g,n} + W_{n-g,n}\right) P_{n+g/m} - \\ - \sum_g \left(W_{n,n+g} + W_{n,n-g}\right) P_{n/m}. \qquad (1)$$

Here $\mathbf{g}$ is the Bravais vectors connecting a given site with the nearest-neighbor along the positive direction of the crystal axes, $W_{n,n+g}$ denotes the transition probability from site $\mathbf{n}$ to the nearest-neighbor site $\mathbf{n} + \mathbf{g}$. In bond disorder system the transition probabilities is given by

$$W_{n,n+g} = \Gamma_{n,n+g} \times f\left(F_g\right), \qquad (2)$$

$$F_g = \beta e E g,$$

where $\beta = 1/k_B T$, e denotes the electronic charge, $\Gamma_{n,n+g} = \Gamma_{n+g,n}$ is the bond disorder transition probability between the nearest-neighbor sites of the lattice. The function f is related to the energy gain or the energy loss during the jump,

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

For simplicity we assume the absence of correlations between the different bonds. The Laplace transform of this equation takes the form

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$$sP_{n/m}(s) = \delta_{n,m} - \sum_g (W_{n,n+g} + W_{n,n-g}) P_{n/m}$$
$$+ \sum_g (W_{n+g,n} + W_{n-g,n}) P_{n+g/m}. \quad (3)$$

The diffusion equation (3) is conveniently represented in matrix forms, using the Dirac formalism:

$$\hat{P} = \sum_{n,n'} P_{n,n'} |n\rangle\langle n'|, \quad (4)$$

$$\hat{V} = \sum_{n,g} \left(\hat{v}^+_{n,g} + \hat{v}^-_{n,g}\right), \quad (5)$$

$$\hat{v}^+_{n,g} = W_{n,n+g} \left(|n+g\rangle - |n\rangle\right) \langle n|$$
$$\hat{v}^-_{n,g} = W_{n+g,n} \left(|n\rangle - |n+g\rangle\right) \langle n+g|, \quad (6)$$

in which the transition rate operators $\hat{v}^{\pm}$ correspond to the forward and backward jumps along the **g**-th direction of the lattice. The basic vectors $|n\rangle$ are orthogonal and form a complete set:

$$\hat{I} = \sum_n |n\rangle\langle n|.$$

Then equation (3) takes the form

$$s\hat{P} = \hat{I} + \hat{V}\hat{P}. \quad (7)$$

The iteration of this equation leads to the infinite series

$$\hat{P} = s^{-1} \sum_{n,g} \left(\hat{v}^+_{n,g} + \hat{v}^-_{n,g}\right) +$$
$$+ s^{-2} \sum_{n,g} \sum_{n',g'} \left(\hat{v}^+_{n,g} + \hat{v}^-_{n,g}\right) \left(\hat{v}^+_{n',g'} + \hat{v}^-_{n',g'}\right) + ... \quad (8)$$

We have to average each term of this expansion with respect to the random distribution of bond disorder transition Γ. In the binary disordered model we use in this paper, the bond strength Γ can take the value Γ_1 with probability c or the value $\Gamma_2 \ll \Gamma_1$, with the probability $1-c$:

$$P(\Gamma) = c\delta(\Gamma - \Gamma_1) + (1-c)\delta(\Gamma - \Gamma_2). \quad (9)$$

The perturbation series thus formally obtained is identical to the lattice models used in the theory of disordered alloys. Using the standard procedure of perturbation theory, one can easy obtain the Dyson equation for the averaged function $\left\langle \hat{P} \right\rangle = \hat{G}$:

$$s\hat{G} = \hat{I} - \hat{W}\hat{G}, \quad (10)$$

where $\hat{G}$ is the Green function describing the diffusion of carriers. The exact summation of the averaged series for the function $\hat{W}$ is impossible. One simple method which can give reasonable results for large disorder is the effective medium approximation (EMA). Using the formal similarity of the series for Green function to the model of binary alloy with diagonal disorder, one can easily obtain an equation for $\hat{W}$ which corresponds to the "coherent potential approximation":

$$\hat{W} = \sum_{n,g} \hat{\sigma}_{n,g}, \quad (11)$$

$$\hat{\sigma}_{n,g} = \langle \hat{v}_{n,g} \rangle + (\hat{v}^1_{n,g} - \hat{\sigma}_{n,g})\hat{G}(\hat{v}^2_{n,g} - \hat{\sigma}_{n,g}), \quad (12)$$

where the operators $\hat{v}^{1,2}$ are obtained from $\hat{v}$ with the replacement $\Gamma = \Gamma_{1,2}$, respectively. As we see from (1) the "coherent potential" $\hat{\sigma}$ has a form similar to $\hat{v}$:

$$\hat{\sigma}_{n,g} = \hat{\sigma}^+_{n,g} + \hat{\sigma}^-_{n,g},$$

$$\hat{\sigma}^+_{n,g} = \sigma^+_g \left(|n+g\rangle - |n\rangle\right) \langle n|, \quad (13)$$

$$\hat{\sigma}^-_{n,g} = \sigma^-_g \left(|n\rangle - |n+g\rangle\right) \langle n+g|.$$

The parameters $\sigma^{\pm}_g$ are connected with each other by a simple relation:

$$\sigma^{\pm}_{n,g} = \sigma_g f(\pm F_g). \quad (14)$$

As a result, we obtain d coupled *self*-consistent equations defining the effective medium transport:

$$\sigma_g = c\Gamma_1 + (1-c)\Gamma_2 + (\Gamma_1 - \sigma)(\Gamma_2 - \sigma) \ \left\{(G_{00} - G_{n+g,n}) f(-F_g) + (G_{00} - G_{n,n+g}) f(F_g)\right\}. \quad (15)$$

Then the Fourier transform of the spatial Green's function $G_{n,n+g}$ is defined by

$$G_{n,n+g}(s) = (2\pi)^{-d} \int \frac{e^{-ikg} dk}{s + \sum_g \sigma_g(s) \left\{[f(F_g) + f(-F_g] (1 - \cos(kg)) + i [f(F_g) - f(-F_g)] \sin(kg)\right\}}, \quad (16)$$

where the integration is over all wave vectors **k** in the first Brillouin zone of the cubic lattice. The steady state drift velocity of a carrier in the effective medium along direction **g** is

$$V_g = \lim_{t\to\infty} \frac{d}{dt} \sum_n G_{0,n} ng/a$$
$$= a\sigma_g(0) \left[f(F_g) - f(-F_g)\right], \quad (17)$$

where a is the lattice constant. The other important characteristic of disordered medium is the diffusion constants. The components of diagonal diffusion tensor are

$$D_{g,g} = \lim_{t\to\infty} \frac{1}{2}\frac{d}{dt}\sum_n G_{0,n}\left[(ng/a)^2 - V_g^2 t^2\right]$$
$$= \frac{a^2\sigma_g(0)}{2}\left[f(F_g) + f(-F_g)\right]. \quad (18)$$

The self consistent equations (15) are similar to the equation obtained recently by Parris and Bookout, except the number of independent parameters [2]. This theory fails to show the negative differential drift velocity associated with bond percolation model in a strong biasing field [2]. The analysis of Shklovskii and co-workers shows that the NDC effect can be identified as arising from "field-induced traps". The latter can be defined as a local configuration of bonds that are easy to enter but difficult to leave, because of hop against the field. It seems reasonable to suggest that effective medium theory which incorporates such "field-induced traps" can be able to describe the effects of NDC.

3. APPLICATION

For further simplification we consider the simple model with combined random traps and random bonds disorder. If these types of disorder are uncorrelated, the resulting drift velocity is factorized into the random-trap and random-bond contributions in one dimension systems [5]:

$$V_{comb} = V_{trap}V_{bond}. \quad (19)$$

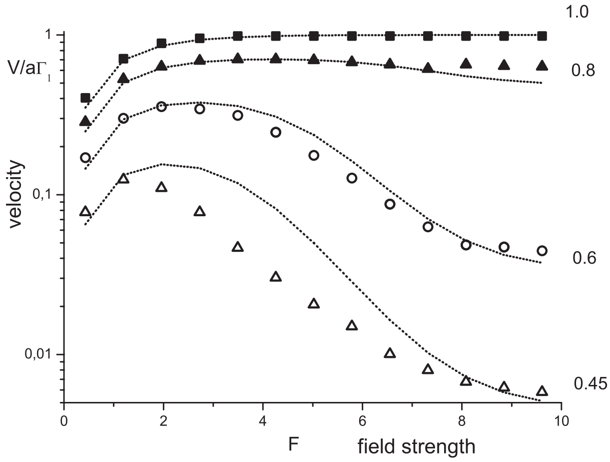
It is plausible to generalize this expression for the random motion on lattice with $d > 1$. Thus, in keeping with the analysis of Ref. [4] we consider bond percolation model where an electrical field $\mathbf{E}$ is directed along the negative direction of the axis X, so that the drift velocity of negative charged carriers is occurred along X axis. Then the simplest trap of this kind is represented by a site with one strong bond along on its left-hand X side, and other $d-1$ bonds being weak, as depicted in the figure. The probability to find such configuration in random lattice is $p = c(1-c)^{d-1}$. The dwelling time at the traps can roughly be estimated as

$$\tau = \left[\Gamma_1 \exp(-F) + (d-1)\Gamma_2\right]^{-1} \quad (20)$$

for the simplest traps, and $F = e\beta Ea$. From (19) and (20) we obtain the following expression for drift velocity along X axis:

$$V_x = \sigma_x\left(1 - e^{-F}\right)\left\langle\frac{a}{\tau}\right\rangle \quad (21)$$
$$= \frac{a\Gamma_1\sigma_x\left(1-e^{-F}\right)}{1 + c(1-c)^{d-1}[\{e^{-F} + (d-1)\Gamma_2/\Gamma_1\}^{-1} - 1]},$$

where for simplicity, we neglect any correlation between the field-induced traps and random bonds. Results of numerical calculations of the drift velocity V_x using (15) and (21) are shown in the figure. Here the drift velocity is presented as a function of the reduced parameter F. The dependences V vs F in the figure are given for the value of weak bonds $\Gamma_2 = 10^{-4}\Gamma_1$ and for various values c of strong bonds above the percolation threshold. The analytical results are compared with Monte Carlo simulation of high field hopping performed by Gartstein and Conwell [4]. We have seen that field-induced traps are responsible for the phenomenon of the NDC in the region of high fields. Of course, real configurations can be more complicated than these simplest traps. But the qualitative picture remains invariable. Our results are no more reliable at the concentration c close to percolation threshold $c \approx 0.25$, where the EMA is not correct.



The dimensionless drift velocity as a function of the reduced field strength F for the model of bond disorder cubic lattice. The value of weak bonds is $\Gamma_2 = 10^{-4}\Gamma_1$. *Data points represent the results of Monte Carlo simulation from Ref. [4]. Dotted lines depict the results of calculation according to the EMA for c =1.0, 0.8, 0.6, and 0.45, respectively*

4. CONCLUSIONS

We have shown that the hopping transport in 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 describe the occurrence of negative differential conductivity in system with bond disorder.

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ПОЛЕВАЯ ЗАВИСИМОСТЬ ПРЫЖКОВОГО ПЕРЕНОСА В СИСТЕМАХ СО СЛУЧАЙНЫМИ БАРЬЕРАМИ

М.П. Фатеев

Развита теория эффективной среды для случая диффузии в однородном внешнем поле с учетом беспорядка связей и случайных радиационно-индуцированных ловушек. Предполагается, что эти величины не коррелируют. Показано, что теоретические результаты хорошо согласуются с моделированием методом Монте-Карло и корректно описывают возникновение отрицательной дифференциальной проводимости в системе с беспорядком связей.

ПОЛЬОВА ЗАЛЕЖНІСТЬ СТРИБКОВОГО ПЕРЕНОСУ У СИСТЕМАХ З ВИПАДКОВИМИ БАР'ЄРАМИ

М.П. Фатеєв

Розвинено теорію ефективного середовища у випадку дифузії в однорідному зовнішньому полі з урахуванням безладдя зв'язків і випадкових радиаційно-індукованих уловлювачів. Передбачається, що ці величини не корелюють. Показано, що теоретичні результати добре узгоджуються з моделюванням методом Монте-Карло і коректно описують виникнення негативної диференціальної провідності в системі з безладдям зв'язків.