Proc. Natl. Conf. Theor. Phys. **37** (2012), pp. 107-114

STUDYING BLOCKING EFFECT FOR MANY PARTICLES DIFFUSION IN ONE-DIMENSIONAL DISORDERED LATTICE

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Abstract. *The diffusion of many particles in one-dimensional disordered lattice has been studied using Monte-Carlo method with periodic boundary conditions. We focus on the influence of energetic disorder and number of particle on diffusivity. The site and transition energies are adopted in accordance to Gaussian distribution. We consider two type lattices: the site disordered lattice (SD); transition disordered lattice (TD). In particular, the blocking effect concerning existence of many particles has been clarified under different temperature and energetic conditions. The simulation results reveal F-effect and τ-effect which affect the diffusivity. As increasing number of particles, the diffusion coefficient DM decreases for both lattices due to F-effect is stronger than τ-effect. The blocking effect is strongly expression as increasing number of particles. For both lattices the blocking effect is almost independent on the temperature.*

I. INTRODUCTION

The diffusion of particles (atom, molecular and ion) in disordered systems (thin-film, amorphous materials, polymers and glasses) has been widely studied for recent decades and received wide attention by many research centres which relates to the field of fuel cells, membrane technology, nano devices [1-10]. Experimental investigations have shown that diffusion in disordered systems has a lot of specific properties such as a strong reduction of the asymptotic diffusion coefficients, anomalous frequency dependence of the conductivity, dispersive transport, etc. The explanation of the diffusion processes in disordered materials has been a challenge to theory. In this work, we probe the diffusion of particles in one-dimensional lattice with site and transition disorders using Monte-Carlo (MC) simulation and analytical method. The particle-particle interaction plays its own role which is interesting and intensively investigated [11-14], but they have no essential relation to the role of energetic disorder and event shadows its influence. Hence, the lattices with non-interacting particles are employed here, and both aspects: energetic disorder and blocking effect, have been studied in two separate systems: the lattice SD where the transition energies are constant but site energies are adopted in accordance to Gaussian distribution [15], and lattice TD that conversely, the transition energies are adopted in accordance to Gaussian distribution and site energies are kept constant.

II. CALCULATION METHOD

Let us consider the hoping of particles between sites in one-dimensional disordered lattice. Each site is characterized by its energy E_i. Hoping of particle to neighboring sites *i-1* and *i+1* is described by transition energy $E_{i,i-1}$ and $E_{i,i+1}$. The transition and site

energies are assigned to each site in a random way from a given distribution Gaussian distribution:

$$p(E) = \frac{1}{\sigma\sqrt{2\pi}} exp(\frac{-(E_x - \mu)^2}{2\sigma^2}) \tag{1}$$

To simply the energy is adopted in accordance to the standard Gaussian distribution with the parameter is given by:

$$p(E) = \frac{1}{\sqrt{2\pi}} exp(\frac{-(E_x)^2}{2}); \qquad with \int_{-5}^{5} p(E) = 1 \tag{2}$$

Here the letter x may be s or t corresponding to the site or transition energy, respectively. Once the particle presents at site i, its probability to hop into neighboring site $i+1$ is given by

$$p_{i,i+1} = \frac{-(E_{i,i+1}\beta)}{(E_{i,j+1}\beta) + E_{i,j-1}\beta} \tag{3}$$

The jump which carries the particle out of site i, is a Poisson process with averaged delay time

$$\tau_i = \frac{2\tau_0 exp(-E_i\beta)}{exp(-E_{i,i+1}\beta) + exp(-E_{i,i-1}\beta)} \tag{4}$$

where τ_0 is frequency period; $\beta = 1/k_B$T;k_B is Boltzmann constant, and T temperature. The time τ_i in fact is the mean residence time of particle on site i. The Monte-Carlo (MC) method is developed mostly for the stationary state and simple form, it does not involve the time. Hence we employed a MC scheme called "residence time" method which can be found elsewhere in [16, 17]. In this method each MC step leads to hop of particle, but random sampling determines the time that particle spent on site i where it visits. After construction of the lattice the sites are filled with N_p particles by randomly choosing their coordinates and avoiding double occupancy. The elementary five steps are:
1/ determine the duration of particle's residence on the current site i by

$$t_{ij} = -\tau_i lnR \tag{5}$$

Initially, a list of time t_{hopj}, j=1, 2,...N_p is determined by equation (5).
2/ select a particle j based on the list t_{hopj}. The particle performing next hop is one that has the earliest time from this list;
3/ select the hop direction of the particle j (to left or right site) according to probability $p_{i,i+1}$ (see Eq. (3))
4/ move the particle j into corresponding neighboring site if this site is non-occupied. Otherwise the particle remains at current site i;
5/ the time t_{hopj} is added to

$$t_{hopj} = t_{hopj} - \tau_i lnR \tag{6}$$

Where R is random number in interval [0,1]. The total duration of the trajectory is given by sum performed along MC steps t_n=$\sum t_{ij}$. The mean time between two consequent jumps equals t_{jumpy}=$\langle t_n \rangle$/n
During simulation the mean square displacement $\langle x_n^2 \rangle$ is obtained by averaging over many runs. Correlation factor F_y is defined in term of the slope of the dependence $\langle x_n^2 \rangle$ vs. n.

Once given a time $\langle t_n \rangle$ that is the averaged duration of n MC steps, the diffusion coefficient can be calculated according to

$$D_y = \frac{a^2}{2} \frac{F_y}{\tau_{jumpy}} \tag{7}$$

Here a is spacing between nearest neighboring sites; τ_{jumpy}=$\langle t_n \rangle$/n is the mean time between two consecutive hops. The letter y may be S, M or C corresponding to single-particle, many-particle and crystal case, respectively. The crystal case corresponds to the lattice where site and transition energies are constant. The simulation has conducted for two types of one-dimensional lattices consisting of 4000 sites with periodic boundary conditions. The values of parameters used for calculation are the same for all simulations: ξ=$\sigma\beta$, $\beta = 1/k_B$T;ξ is dimensionless and varies in the interval from 0.2 to 2. The averaged number of hops per particle is n = 1000; The number of particles is varies varies interval from 1 to 120 particles. In order to attain a good statistic all quantities is obtained by averaging over 10^6 MC samplings.

III. RESULT AND DISCUSSION

III.1. The single-particle case

Figure 1 shows the factor F_S, the ratio $\tau_{jumpS}/\tau_{jumpC}$, D_S/D_C as function of temperature. For SD lattice one finds the correlation factor F_S does not depend on temper-

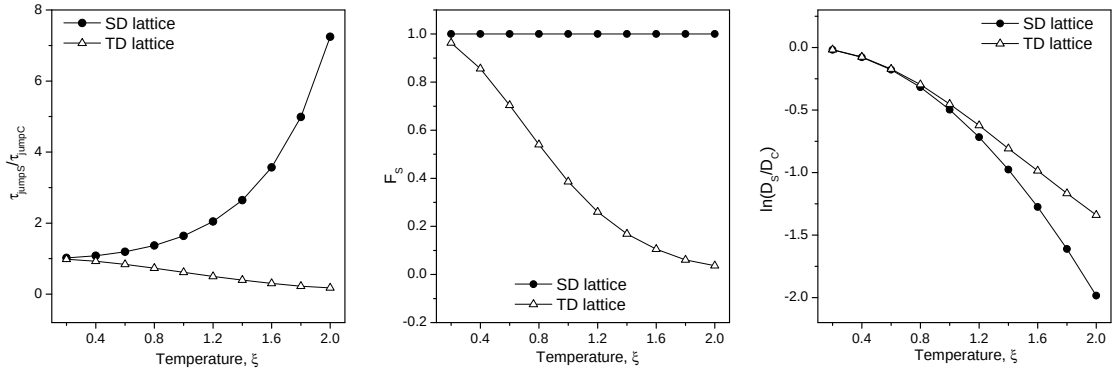

Fig. 1. The dependence of $\tau_{jumpS}/\tau_{jumpC}$, correlation factor F_S and $\ln(D_S/D_C)$ on temperature for SD, TD lattices

ature and is approximately equal to 1, the time $\tau_{jumpS}/\tau_{jumpC}$ increases as temperature decreases (i.e. ξ increases). Furthermore, comparing to TD lattice the correlation factor decreases strongly as temperature decreases and the time $\tau_{jumpS}/\tau_{jumpC}$ of SD lattice is significantly larger than one of TD lattice indicating the specific properties of trapping model (SD) in comparison with hoping model (TD). The result of diffusion coefficient is also presented in figure 1. The simulated results showed that the ratio D_S/D_C decreases with temperature. The ratio D_S/D_C of TD lattice is very close to one of SD lattice if both lattices have the same temperature interval from 0.2 to 1.4 and identical distribution

of barriers although the character of particles motion in them is quite different. However, in the low temperature interval ($\xi > 1.2$) this result is not true.

III.2. Many - particles case

Table 1. The diffusion quantities for many-particles at $\xi = 1.4$ and $n = 1000$. Here n is averaged number of hops per particle; n_{high}, n_{low} are the averaged number of visit to site with high and low energy, respectively; $n_{high} + n_{low} = n$; n_{uns} is number of unsuccessful jumps; $\tau_{MC} = \tau_{jumpM}/\tau_{jumpC}$.

Lattice	N	n_{high}	n_{low}	n_{uns}	n_{uns}/n	F_M	τ_{MC}	D_M/D_C
SD	1	699.43	301.57	0	0	1.001	2.648	0.376
	10	698.7	301.4	0.42	0.00042	0.938	2.588	0.358
	20	699.97	300.08	0.92	0.00092	0.874	2.559	0.338
	40	702.49	297.54	1.92	0.00192	0.764	2.506	0.302
	60	705.15	294.87	2.98	0.00298	0.672	2.457	0.271
	80	707.53	292.49	4.06	0.00406	0.595	2.417	0.244
	120	712.39	287.62	6.36	0.00636	0.473	2.337	0.200
TD	1	-	-	0	0	0.169	0.397	0.446
	10	-	-	2.25	0.00225	0.166	0.380	0.439
	20	-	-	4.76	0.00476	0.160	0.377	0.427
	40	-	-	9.79	0.00979	0.152	0.377	0.403
	60	-	-	14.87	0.01487	0.143	0.377	0.381
	80	-	-	19.88	0.01988	0.136	0.378	0.361
	120	-	-	29.77	0.02977	0.122	0.377	0.324

In case of many - particles, the blocking effect plays a relevant role. Unlike single-particle case, some particles jumps in many-particles case are suppressed due to that a number of sites are occupied, which does not lead to particles displacement. Obviously the number of such jumps (unsuccessful hop) n_{uns} increases with the number of particles. Consequently, the mean square displacement and correlation factor F_M decreased with increasing number of particles. Table 1 presents the diffusion quantities for many-particles case at ξ =1.4. The number nuns relates to the correlation factor F_M . As increasing number of particles the n_{uns}/n increases 15.14 times for SD lattice and 13.23 times for TD lattice, meanwhile the factor F_M decreases for both SD (1.99 times) and TD (1.36 times) lattices. This effect is denoted to F-effect. This effect can be explained as follows: since the particles hop is unsuccessful, the probability that the particles hop in opposite direction becomes bigger than one in original direction. This gives rise to increasing the number of forward-backward hops and results in that F_M is decreased and it decreases the diffusion coefficient D_M. Furthermore, for SD lattice the mean particles residence time for the site with low energy is larger than one for site with high energy. Therefore, the occupied site with low energy prevents other particles to jump into it by lager time than the occupied site with high energy. As a result, due to blocking the averaged number of particles visit to the site with low energy decreases with the number of particles. This in turn leads to decreasing mean time between two consecutive hops τ_{jumpM}. This effect is called τ-effect.

This second effect increases D_M. For TD lattice the particle spent in average the same time for each site. However, it prefers to surmount the saddle point with low transition energy. Hence the particles jumps over the saddle point with low transition energy are more frequent than ones over saddle point with high transition energy. As a result, due to blocking the number of jumps over saddle point with low transition energy when the number of particles is enough lager. This in turn increases time τ_{jumpM}. Nevertheless, our simulation results show that τ_{jumpM} decreases (see Table 1). This can be explained as follows: in the considered number of particles interval (from 10 to 120 particles) the blocking effect is weekly for TD lattice due to the number of particles is not enough large. As expected, the number nhigh and nuns increases monotonously as the number of particles increases from 10 to 120. This gives rise to decreasing F_M and τ_{jumpM}. However, as shown table 1 the D_M/D_C decreases with number of particle for all considered lattices. It implies that for 1D lattice first effect (F-effect) is stronger than second one (τ-effect). Figure 2 shows that the dependence of correlation factor F_M on temperature for SD and TD lattices. Similar to in case of single-particle, for SD lattice the factor F_M is independent

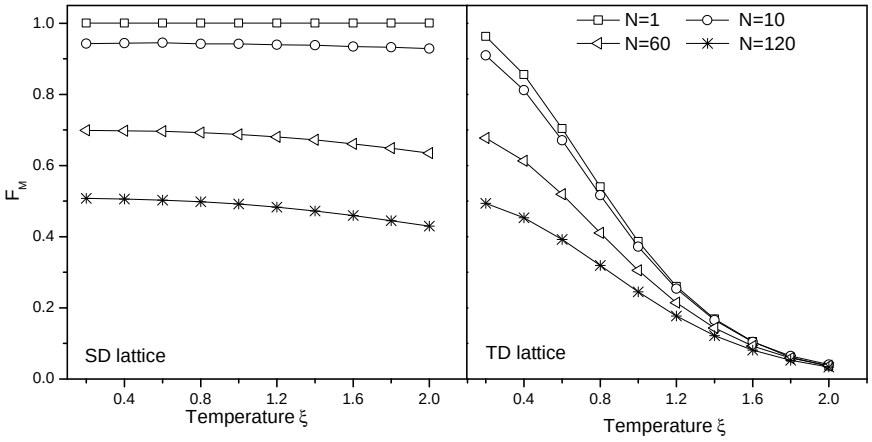

Fig. 2. The dependence of correlation factor F_M on temperature for SD, TD lattices

of temperature but for TD lattice the factor F_M is strongly dependent of temperature and decreases with temperature. To give additional insight into the many-particle effects we studied the temperature dependence of quantity $\ln(D_M/D_C)$ shown in Figure 3. As shown in this figure, the diffusion does not follow Arrhenius law for all cases. In accordance to ref. [16] the Arrhenius behavior for diffusion in amorphous material is caused by the compensation between site and transition disordered. This discrepancy may be related to the finite energetic distribution used in [16]. To estimate the strength of blocking effect we have calculated the ratio F_M/F_S, $\tau_{jumpM}/\tau_{jumpS}$, D_M/D_S which are shown in figure 4. It can be seen that F_M/F_S decreases with different rate depending on the type of disorder and number of particles. Meanwhile for TD lattice $\tau_{jumpM}/\tau_{jumpS}$ is almost unchanged or slightly increases with number of particles, for SD lattice its value strongly decrease at

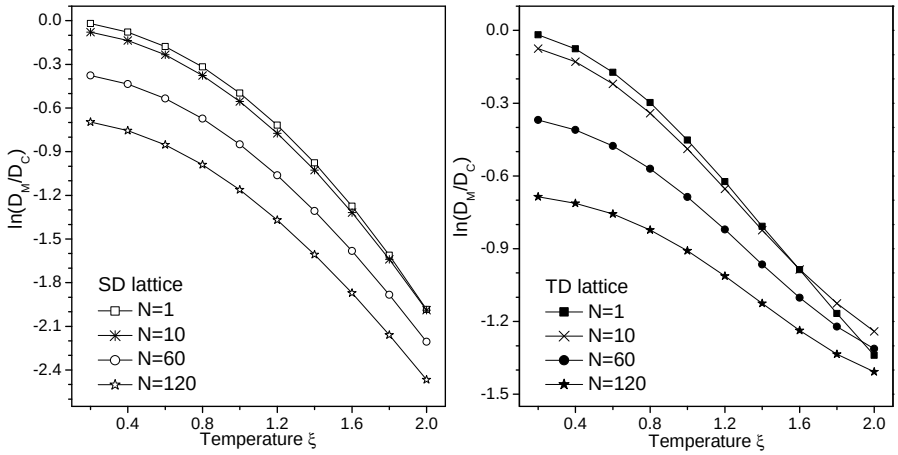

Fig. 3. The dependence of $\ln(D_M/D_C)$ on temperature for SD, TD lattices

=1.4; The D_M/D_S decreases with number of particles for both SD and TD lattice. As such, increasing number of particles is accompanied with two effects: F-effect decreases D_M and τ-effect increases D_M. However, for TD lattice F-effect is mainly but for SD lattices F-effect is stronger than τ-effect. Figure 5 shows the temperature dependence of

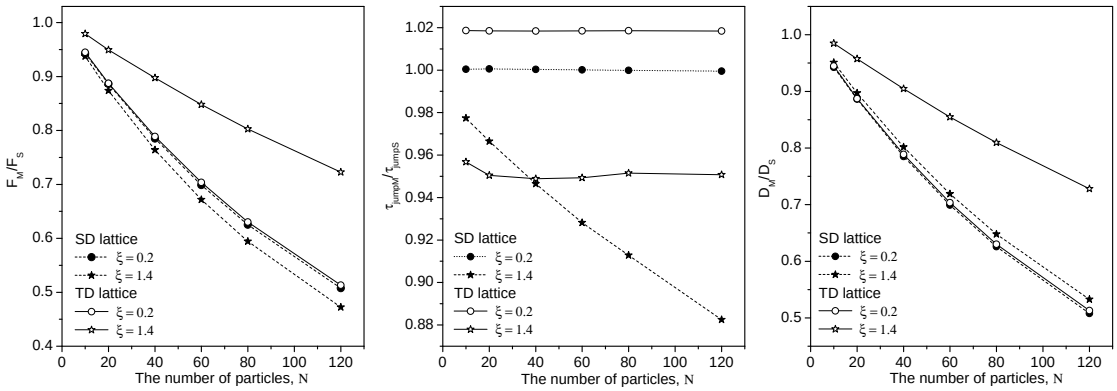

Fig. 4. The dependence of $\tau_{jumpM}/\tau_{jumpS}$, correlation factor $F_M/F_S$and $\ln(D_M/D_S)$ on the number of particles for SD, TD lattices

F_M/F_S, $\tau_{jumpM}/\tau_{jumpS}$, D_M/D_S for SD and TD lattice. The dependence for F_M/F_S as well as for $\tau_{jumpM}/\tau_{jumpS}$ is quite different between SD and TD lattice. In the considered temperature interval the ratio F_M/F_S decreases from 0.507 to 0.429 for SD lattice; whereas, it increases from 0.513 to 0.927 for TD lattice. Despite that the factor F_M as well as the time τ_{jumpM} strongly depends on the temperature, the ratio D_M/D_S weakly changes in the considered temperature interval. Therefore, the blocking effect weakly depends on the

temperature.

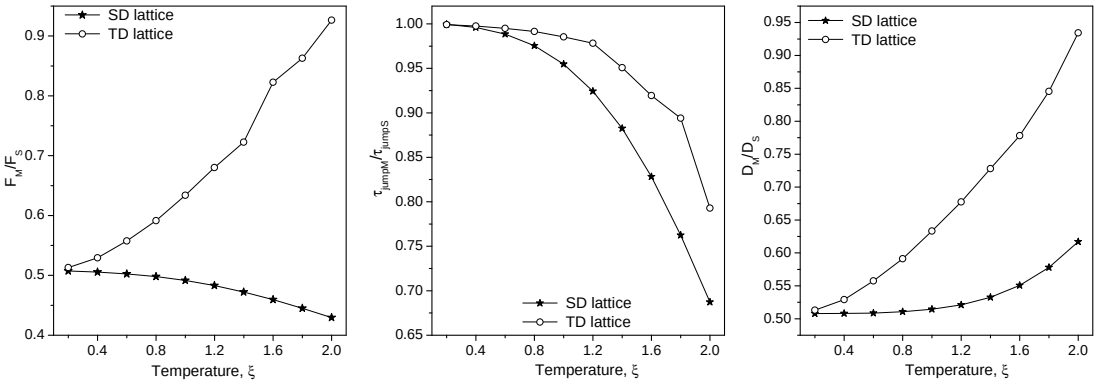

Fig. 5. The dependence of $\tau_{jumpM}/\tau_{jumpS}$, correlation factor $F_M/F_S$and $\ln(D_M/D_S)$ on temperature for SD, TD lattices

IV. CONCLUSION

Monte-Carlo has been simulation carried out for the diffusion in one-dimensional disordered lattices with Gaussian distributions of site and transition energies. The mainly conclusions in this work can be done as follow:
1/ The simulation for many-particles case reveals two specific effects: F-effect and τ-effect. As increasing number of particles, the diffusion coefficient D_M decreases for SD and TD lattices due to F-effect is stronger than τ-effect.
2/ The Arrhenius behavior is not observed for all considered lattices.
3/ We have demonstrated that blocking effect is strongly dependent number of particles but is weakly dependent with the temperature. In the considered number of particles interval (from 10 to 120 particles) the blocking effect in SD lattice is more expression than TD lattices. The more number of particles is larger the more blocking effect is expression.

ACKNOWLEDGMENT

This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.99-2011.22.

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Received 30-09-2012.