

# Diffusion of interacting particles in one-dimensional heterogeneous systems

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## Abstract

The equilibrium and transport properties of interacting ad-particles on bivariate heterogeneous chains are studied by combining analytical and simulation approaches. Heterogeneity is introduced in the way of patches of shallow and deep adsorbing sites distributed in a deterministic alternating way. Adsorption isotherms and mean-square fluctuations of the surface coverage, as well as the jump and collective diffusion coefficients, are calculated for different values of lateral interactions between ad-particles and substrate heterogeneity. In addition, different elementary jump mechanisms are introduced and their influence in the coverage dependence of the collective diffusion coefficient is investigated.

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## 1. Introduction

It is already some time since low-dimensional systems are no more a curiosity or an abstraction in nature and have won also a practical interest due to the fact that they are effectively realized in many real situations [1–6]. In particular, one-dimensional systems appear in a variety of phenomena, as different as, for example, the kinetics of laser-induced excitons in TMMC crystals [1], conduction in quantum wires [2,3] or the behavior of particles adsorbed in carbon nanotubes [4–6]. Another source of interest in these low-dimensional systems is that it is not unusual to find that many processes (for example reaction–diffusion processes) may present novel behaviors as compared to the same processes in higher dimensions [7].

Processes in low-dimensional systems may be affected by heterogeneity (i.e., the properties of the system present spa-

tial variations), which, as in higher-dimensional systems, is usually present in real materials. Just as a simple example, the helicoidal winding of graphite planes in a carbon nanotube may determine adsorbing sites of different energies along the axis. More complex heterogeneities may arise through the presence of defects or impurities in the material.

Previous studies have preferentially addressed equilibrium properties of ad-particles in heterogeneous one-dimensional systems [8–10]; however kinetic properties, in particular diffusion, are perhaps as important as the former. Our purpose here is therefore to study, by using Monte Carlo simulations, the diffusion of interacting ad-particles in one-dimensional heterogeneous systems, where heterogeneity is introduced by considering the system as composed by an alternating collection of patches of shallow and deep adsorbing sites. In addition to the effects of lateral interactions and of the degree of heterogeneity, we are also interested in studying the effects of different jumping rules, since it is to be expected that in a one-dimensional system diffusion will be more sensitive to such rules. In the case of homogeneous surfaces, Monte Carlo

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simulations are compared with theoretical results, in the framework of a lattice-gas model derived phenomenologically by Reed and Erlich [11,12]. Despite the limitations of the model an excellent agreement is obtained in all studied cases.

It is worth noticing that although lateral interactions are introduced in the present model, the system does not show a phase transition at finite temperature (it is well-known that no phase transition develops in a one-dimensional lattice when weak coupling between neighboring particles exists). If interactions are important and phase transitions are possible, modeling diffusion becomes significantly harder. In this sense, important approaches to diffusion of interacting particles have been recently reported. Among them, Giacomini et al. [13–15] developed a rigorous statistical mechanical theory of nonequilibrium phase transitions. This theory provides a fundamental theoretical background for modeling the evolution of nonequilibrium coexisting phases. More recently, a new approach to molecular diffusion of interacting particles was developed by Aranovich and Donohue [16]. The calculations were derived using density functionals for fluxes and the Metropolis algorithm in the mass balance equation.

The paper is organized as follows. In Section 2 we will introduce the physical model and develop both exact analytical solutions for homogeneous systems and Monte Carlo simulations for the general heterogeneous system. Results are presented and discussed in Section 3 and, finally, conclusions are given in Section 4.

## 2. Basic formulation

### 2.1. The model

We consider the adsorption of simple particles on a one-dimensional heterogeneous bivariate lattice. The substrate is represented by a chain of  $M$  adsorptive sites with periodic boundary conditions. Heterogeneity is introduced by considering two kinds of adsorptive sites, deep and shallow traps, in equal concentrations ( $f_D = f_S = 0.5$ ), with adsorption energies given by  $\epsilon_D$  and  $\epsilon_S$ , respectively, spatially distributed as alternating patches of size  $l$ , as shown in Fig. 1.

In order to describe the system of  $N$  particles adsorbed on  $M$  sites (each site can only be empty or occupied by a single particle) at a given temperature  $T$ , we use the occupation variable  $c_i$  (equal to zero if site  $i$  is empty or equal to 1 if occupied) and define the Hamiltonian of the system as

$$H = w \sum_{(i,j)} c_i c_j + \sum_{i=0}^M c_i \epsilon_i - \mu \sum_{i=0}^M c_i \quad (1)$$

where  $w$  is the lateral interaction among nearest-neighbor (NN) particles,  $(i,j)$  represent all pairs of NN sites and  $\mu$  is the chemical potential.

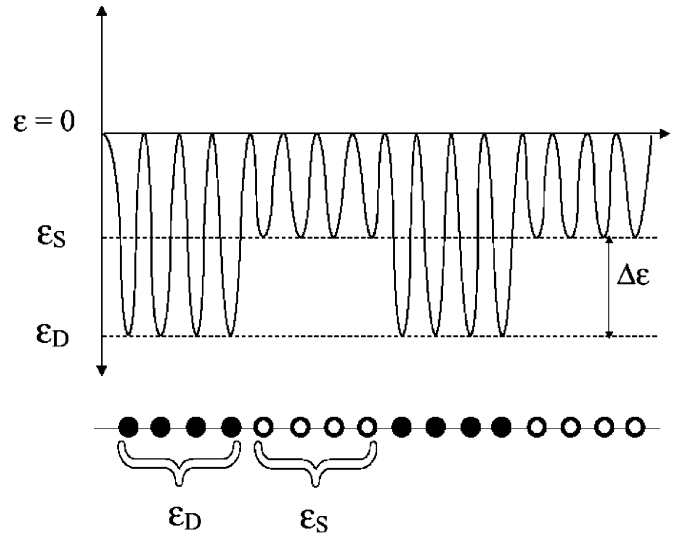


Fig. 1. Schematic representation of a one-dimensional bivariate surface with patchwise topography. The filled (empty) circles represent the deep (shallow) sites with energy  $\epsilon_D$  ( $\epsilon_S$ ). The patch size in the figure is  $l = 4$ .

We consider that particles can jump to NN empty sites through one of the two following elementary transitions: the normal activated transition (AT), where the transition rate depends only on the initial particle configuration, and a “tunnel-like” transition (TT), where the transition rate depends both on the initial and final particle configurations. The four elementary hopping processes are schematically given in Fig. 2, representing the hopping from an occupied (●) to an empty (○) site when this pair of sites is immersed in all possible environments. To be specific, we define for these two transitions the following hopping rates for a (●○) pair of sites immersed in an environment  $i$ :

$$k_{\bullet\circ,i}^{AT} = v \exp[-(\epsilon_i^* - \epsilon_{\bullet\circ,i})/k_B T] \quad (2)$$

$$k_{\bullet\circ,i}^{TT} = \begin{cases} v \exp[-(\epsilon_{\circ\bullet,i} - \epsilon_{\bullet\circ,i})/k_B T] & \text{if } (\epsilon_{\circ\bullet,i} - \epsilon_{\bullet\circ,i}) > 0 \\ v & \text{otherwise} \end{cases} \quad (3)$$

where  $v$  is a pre-exponential factor,  $\epsilon_i^*$  is the lateral interaction of the activated complex with the environment  $i$ ,  $\epsilon_{\bullet\circ,i}$  is the energy of the (●○) pair in the environment  $i$ , and so on.

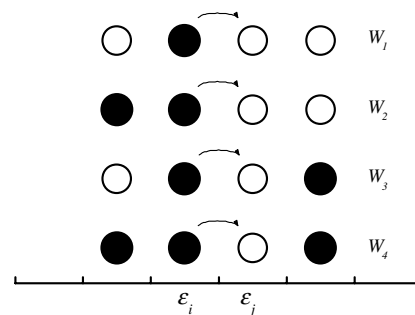


Fig. 2. Elementary hopping processes. Full and empty circles represent particles and vacancies, respectively.

### 2.2. Exact equilibrium solution for a homogeneous chain

It is instructive to derive the exact solution for the particular case of a homogeneous chain where  $\varepsilon_D = \varepsilon_S = 0$ . In addition, such a solution can be used to test the Monte Carlo simulation method to be developed below to study the general heterogeneous case.

The exact form of the free energy per site,  $f$ , was obtained explicitly in Refs. [17,18] as a function of  $T$  and the coverage  $\theta = N/M$ :

$$\begin{aligned} f(\theta, T) &= \frac{F(M, N, T)}{M} \\ &= w(\theta - \alpha) - k_B T [\theta \ln \theta + (1 - \theta) \ln(1 - \theta) \\ &\quad - 2\alpha \ln \alpha] + k_B T [(\theta - \alpha) \ln(\theta - \alpha) \\ &\quad + (1 - \theta - \alpha) \ln(1 - \theta - \alpha)] \end{aligned} \quad (4)$$

where

$$\alpha = \frac{2\theta(1 - \theta)}{1 + b}; \quad b = [1 - 4(1 - e^{-w/k_B T})(\theta - \theta^2)]^{1/2} \quad (5)$$

All equilibrium properties of the system can be obtained from Eq. (4) along with the differential form of  $F$  in the canonical ensemble:

$$dF = -S dT - \Pi dM + \mu dN \quad (6)$$

where

$$S = -\left(\frac{\partial F}{\partial T}\right)_{M,N}; \quad \Pi = -\left(\frac{\partial F}{\partial M}\right)_{T,N}; \quad \mu = \left(\frac{\partial F}{\partial N}\right)_{M,T} \quad (7)$$

In particular, the coverage dependence of the chemical potential and the entropy per site,  $s$ , are obtained as

$$\mu(\theta, T)/k_B T = w/k_B T + \ln(b - 1 + 2\theta) - \ln(b + 1 - 2\theta) \quad (8)$$

$$\begin{aligned} s(\theta, T)/k_B &= \theta \ln \theta + (1 - \theta) \ln(1 - \theta) - 2\alpha \ln \alpha \\ &\quad - (\theta - \alpha) \ln(\theta - \alpha) - (1 - \theta - \alpha) \ln(1 - \theta - \alpha) \end{aligned} \quad (9)$$

To study the transport process we follow the framework of the theoretical approach derived phenomenologically by Reed and Ehrlich [11,12,19]. In this model, equilibrium grand canonical distribution is used for calculation of probabilities of jumps which is equivalent to the hypothesis of local equilibrium. Under these considerations, the collective diffusion coefficient,  $D(\theta)$ , is written as

$$D(\theta) = D(0)\Phi \exp(\mu/k_B T) \left(\frac{\partial \mu/k_B T}{\partial \theta}\right)_T \quad (10)$$

$$\Phi = \sum_{i=1}^{\gamma} P_{\circ\circ,i} k_{\bullet\circ,i} \exp(-\varepsilon_{\bullet\circ,i}/k_B T) \quad (11)$$

where  $D(0)$  is the diffusion coefficient in the limit of zero coverage,  $P_{\circ\circ,i}$  is the probability of an empty pair of sites in an environment  $i$  and  $\gamma$  is the total number of different environments.

Coefficient  $\Phi$  depends on which of the two transition processes, given in Eqs. (2) and (3), are being considered. For an AT process we have:

$$\Phi^{AT} = \sum_{i=1}^{\gamma} P_{\circ\circ,i} \exp(-\varepsilon_i^*/k_B T) \quad (12)$$

In the particular case where the activated complex does not interact with the environment,  $\varepsilon_i^* = 0$  and we obtain simply:

$$\Phi^{AT} = \sum_{i=1}^{\gamma} P_{\circ\circ,i} = P_{\circ\circ} \quad (13)$$

For a TT process, on the other hand, and separating the sum in terms of each contributing environment, we obtain:

$$\begin{aligned} \Phi^{TT} &= P_{\circ\circ\circ\circ} k_{\circ\circ\circ\circ}^{TT} \exp(-\varepsilon_{\circ\circ\circ\circ}/k_B T) + P_{\bullet\circ\circ\circ} k_{\bullet\circ\circ\circ}^{TT} \\ &\quad \times \exp(-\varepsilon_{\bullet\circ\circ\circ}/k_B T) + P_{\circ\circ\circ\bullet} k_{\circ\circ\circ\bullet}^{TT} \\ &\quad \times \exp(-\varepsilon_{\circ\circ\circ\bullet}/k_B T) + P_{\bullet\circ\circ\bullet} k_{\bullet\circ\circ\bullet}^{TT} \\ &\quad \times \exp(-\varepsilon_{\bullet\circ\circ\bullet}/k_B T) \end{aligned} \quad (14)$$

By using Eqs. (8) and (10)–(14), together with the expressions for all the involved configurational probabilities given in Ref. [20], the collective diffusion coefficient can then be calculated.

### 2.3. Monte Carlo simulation of adsorption

For heterogeneous systems exact analytical solutions are not available and some other convenient method, like Monte Carlo simulation, must be used. The adsorption process is conveniently simulated in the Grand Canonical Ensemble [21]. For a given value of the temperature and the chemical potential, an initial configuration with  $N = M/2$  particles adsorbed at random positions is generated. Then, an adsorption–desorption chain of events is started by choosing a site at random and attempting to change its occupancy number according to the Metropolis transition probability [22]:

$$P = \min \left\{ 1, \exp \left( -\frac{\Delta H}{k_B T} \right) \right\} \quad (15)$$

where  $\Delta H = H_f - H_i$  is the difference between the Hamiltonians of the final and initial states. A Monte Carlo step (MCS) is achieved when  $M$  sites have been tested to change their occupancy state. The approximation to thermodynamic equilibrium is monitored through the fluctuations in the number  $N$  of adsorbed particles; this is usually reached in about  $10^5$  MCS. After that averages are taken on the system through the next  $10^5$  MCS on non-correlated configurations. At high values of  $w/k_B T$  up to  $10^6$  MCS had to be used in order to let the system to relax from metastable states.

Thermodynamic quantities such as the mean coverage,  $\bar{\theta}$ , and the mean energy,  $\bar{U}$ , are obtained as simple averages:

$$\bar{\theta} = \frac{1}{M} \sum_{i=1}^M \langle c_i \rangle; \quad \bar{U} = \langle H \rangle \quad (16)$$

where the bracket denotes average over  $n$  uncorrelated configurations. The thermodynamic factor,  $T_h$ , is calculated through the average:

$$T_h = \left[ \frac{\langle \delta N \rangle^2}{\langle N \rangle} \right]^{-1} \quad (17)$$

and is equivalent to the factor:

$$T_h = \left[ \frac{\partial(\mu/k_B T)}{\partial \ln \theta} \right]_T \quad (18)$$

involved in the calculation of the collective diffusion coefficient.

#### 2.4. Monte Carlo simulation of diffusion

Since we are interested in describing diffusion of ad-particles at constant coverage, Monte Carlo simulations for this process will be performed in the Canonical Ensemble, where the number  $N$  of particles is kept constant. Diffusion jumps are allowed only to NN empty sites and take place through one of the two above described mechanisms, AT and TT mechanisms.

The method for determining the *collective diffusion coefficient*,  $D(\theta)$ , is based on the Kubo–Green equation which we write here as [11,12,23]:

$$D(\theta) = D^J(\theta) \left( \frac{\partial \mu / k_B T}{\partial \ln \theta} \right)_T \quad (19)$$

where  $D^J(\theta)$  denotes the *jump diffusion coefficient* representing the time dependence of the mean square displacement of the center of mass of particles,  $\langle R^2(t) \rangle$ . For the diffusion of simple (monomer) particles in one dimension it is known that  $\langle R^2(t) \rangle \propto t$  [9,24], so that the jump diffusion coefficient can be easily obtained from simulations through:<sup>1</sup>

$$D^J(\theta) = \lim_{t \rightarrow \infty} \frac{\langle R^2(t) \rangle}{2t} \quad (20)$$

Our numerical simulations are performed by considering a fast kinetic Monte Carlo scheme based on the  $n$ -fold way-like algorithm ( $n$ FWMC) [9,24,25], which relies on the exact computation of the transition probabilities from each configuration of the system and the association of the time evolution to a random variable sampled from the waiting time distribution for these configurations. Therefore, the Monte Carlo simulation of the diffusion process is performed by iterating the following two steps for any given configuration:

- (i) The transition probabilities,  $W_i$  ( $i = 1, 2, \dots, 2N$ ), where  $2N$  is used to account for the two possible transitions (to the left or to the right) for each particle, are evaluated by using Eqs. (2) and (3). Then, a random number  $\xi_1$  uniformly distributed in  $(0, 1)$  is obtained and the  $k$ th event chosen from the condition:

$$\frac{1}{W} \sum_{i=1}^{k-1} W_i < \xi_1 \leq \frac{1}{W} \sum_{i=1}^k W_i; \quad W = \sum_{i=1}^{2N} W_i \quad (21)$$

is performed.

- (ii) A second random number  $\xi_2$  is generated and the time  $t$  elapsed from the initial state is incremented through:

$$t = t + \Delta t = t - \frac{1}{W} \ln \xi_2 \quad (22)$$

The advantage of using the  $n$ FWMC scheme described above can be understood by taking into account that in the standard kinetic Monte Carlo simulation framework the number of trials for a successful jump scales as a function of time as  $1/W_i$ , while the efficiency of  $n$ FWMC is not affected by an increase in  $w/k_B T$  or  $\varepsilon_i/k_B T$ , since every trial produces a successful jump of some particle to a NN empty site.

### 3. Results and discussion

Our simulations were performed for lattices with  $M = 4000$ ,  $l = 4$  and periodic boundary conditions; under these conditions we verified that finite size effects are negligible. The jump diffusion coefficient was determined in the Canonical Ensemble by fitting the curves  $R^2(t)$  for long times, when the asymptotic regime is reached. This, and the calculation of the thermodynamic factor obtained from simulations in the Grand Canonical Ensemble, allows the calculation of the collective (or chemical) diffusion coefficient through the Kubo–Green formula.

As a basis for discussing the effects of heterogeneity, we begin by briefly reviewing the results corresponding to the particular case of a homogeneous chain. The coverage dependence of the chemical potential (adsorption isotherm) and the thermodynamic factor are shown in Fig. 3(a) and (b), respectively, for different values (attractive and repulsive) of the lateral interaction energy. The isotherms present a characteristic pronounced plateau at  $\theta = 0.5$  for large repulsive values of  $w/k_B T$ , accompanied by a sharp peak in the thermodynamic factor. Fig. 4 shows the normalized jump diffusion coefficient,  $D^J(\theta)/D^J(0)$ , for the TT (a) and AT (b) mechanism, and the normalized collective diffusion coefficient, for the TT (c) and AT (d) mechanism. The most relevant characteristics is the sharp minimum in  $D^J$ , and sharp maximum in  $D$ , at  $\theta = 0.5$  where a frozen structure is formed for repulsive interactions. The excellent agreement between symbols (Monte Carlo results) and lines (exact calculations) reinforces the validity of the simulation method.

<sup>1</sup> It is worth noticing that our discussion concerned with the jump and chemical diffusion coefficients is valid for lattices with one or more spatial dimensions. However, the tracer diffusion of particles in one dimension leads to  $\langle R^2(t) \rangle \propto \sqrt{t}$  for the mean square displacement of single particles, so that the tracer diffusion coefficient,  $D^*$ , is strictly zero in one dimension. Our Monte Carlo simulations show that  $\langle R^2(t) \rangle \propto t$  for the mean square displacement of the center of mass. Thus  $\langle R^2(t) \rangle = 2dD^J t$  and  $D^J$  is meaningful in the present case.

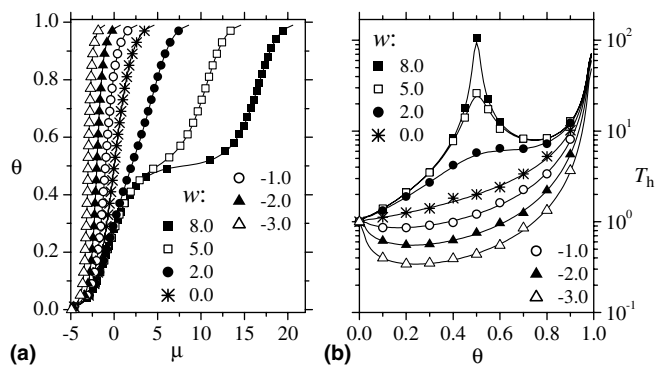


Fig. 3. Comparison between exact theoretical results (solid lines) and Monte Carlo simulations (symbols) for interacting particles adsorbed on homogeneous chains: (a) adsorption isotherms, (b) thermodynamic factors.

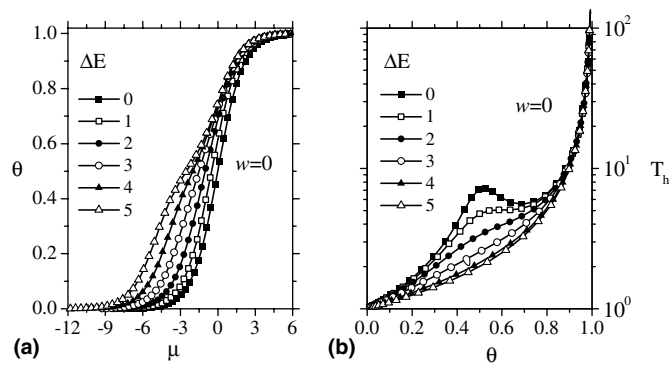


Fig. 5. Effect of surface heterogeneity  $\Delta E$  on adsorption isotherms (a) and thermodynamic factors (b) for non-interacting particles.

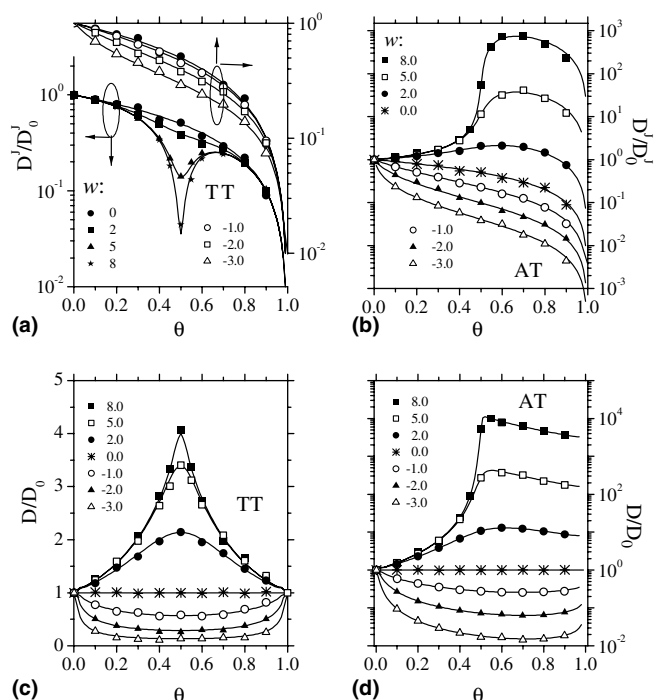


Fig. 4. Jump (a and b) and collective (c and d) diffusion coefficient for interacting particles on homogeneous chains for TT and AT jumping mechanism, respectively.

Proceeding to a more complex situation, we now study the effects of heterogeneity in absence of lateral inter-particles interactions,  $w=0$ . Figs. 5 and 6 show the results for different values of the heterogeneity strength,  $(\epsilon_D - \epsilon_S)/k_B T = \Delta E$ . The adsorption process separates into two regimes as  $\Delta E$  increases: deep sites are occupied first and then the rest of the lattice is filled [26], this results in a shoulder in adsorption isotherms (Fig. 5a) and a maximum in the thermodynamic factor (Fig. 5b). It can be verified that  $T_h$  exhibits the well known behavior given by  $1/(1 - \theta)$  for the homogeneous case,  $\Delta E = 0$ . The behavior of the jump diffusion coefficient is, as it also happened for the homogeneous case, quite different for the TT and

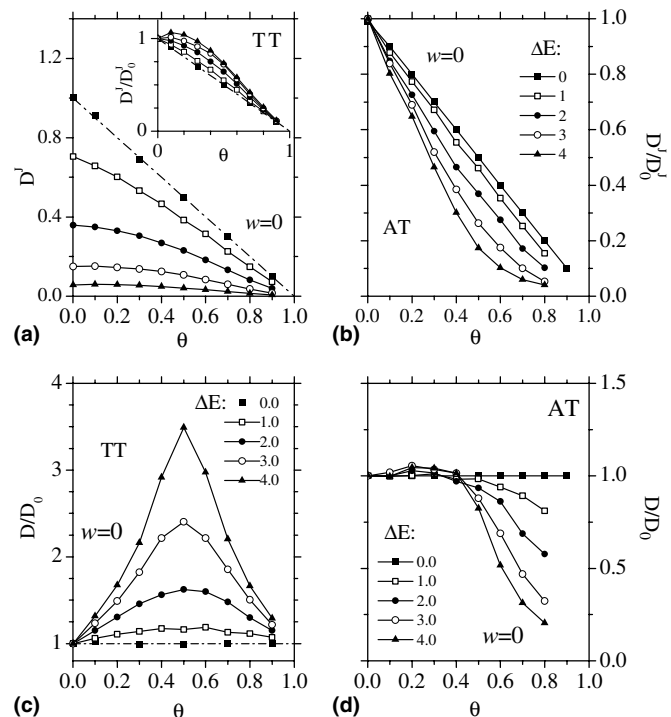


Fig. 6. Jump (a and b) and collective (c and d) diffusion coefficient for non-interacting particles on homogeneous chains for TT and AT jumping mechanism, respectively.

AT mechanisms (Fig. 6a and b). Here, since  $D_0^J$  depends on  $\Delta E$ , it is convenient to analyze  $D^J$  (main graphic) in addition to  $D^J/D_0^J$  (inset). For  $\Delta E = 0$  both mechanisms show the exact  $(1 - \theta)$  dependence of the homogeneous case. As heterogeneity increases  $D^J$  decreases, however it decreases much slower (both as a function of  $\Delta E$  and as a function of  $\theta$ ) for TT than for AT. Even more, at low coverage and high values of  $\Delta E$ , the jump diffusion coefficient for TT presents a maximum, which can be better appreciated in the inset of Fig. 6a. The explanation of this behavior is as follows. For AT, particles crossing the boundary between patches in a given direction can take during the next jump either the backward or the forward direction with the same probability, therefore there is no

trapping effect on any patch. Nevertheless, in this mechanism jumps inside a deep patch are slower than those inside shallow patches (and in both cases they are slower than for TT). This results in a fast decay of  $D^J$  as a function of  $\Delta E$  and  $\theta$ . For TT, on the contrary, if a particle jumped across a patch boundary from a shallow patch to a deep one, the probability for a backward jump is lower than that for a forward jump and particles tend to get trapped in the deep patches. However, the jumping rate on a deep patch is fast (in fact equal to  $v$ , the same as the jumping rate on a shallow patch). Therefore, at low coverage (say  $\theta \sim 0.2$ ) the system is in a configuration where particles are distributed preferentially on the alternating deep patches, with 1 or at most 2 particles per patch, and these particles are jumping rapidly inside each patch producing an enhancement of  $D^J$ .

The combination of the effects just discussed for  $T_h$  and  $D^J$  produces the behavior of the collective diffusion coefficient shown in Fig. 6c and d. Here we can see that the difference in the coverage dependence of  $D/D_0$  for TT and for AT is much more important than for the jump diffusion coefficient. In particular, there is a sharp peak and symmetry around  $\theta = 0.5$  for TT. It is interesting to note that, due to the qualitatively different behavior, it may become possible to obtain information on the jumping mechanism (an important microscopic knowledge of the system) from experimental observations of the diffusion coefficient.

Finally, in order to complete the study the combined effect of heterogeneity and lateral interactions is considered. We divide the results in two parts, for repulsive (Figs. 7 and 8) and for attractive (Figs. 9 and 10) interactions, both for a fixed value of heterogeneity  $\Delta E = 2$ . In each case the results can be readily interpreted by adding the separate effects of heterogeneity and lateral interactions discussed in detail above. The behavior of the jump diffusion coefficient for attractive interactions is similar both for the TT and AT mechanisms, and is monotonically decreasing with coverage, as it can be readily understood. However, significant qualitative differences arise for repulsive interactions. In this case, near  $\theta = 0.5$  where an ordered structure is formed on each homogeneous patch, the system becomes nearly frozen for the TT mechanism, due to the fact that any jump

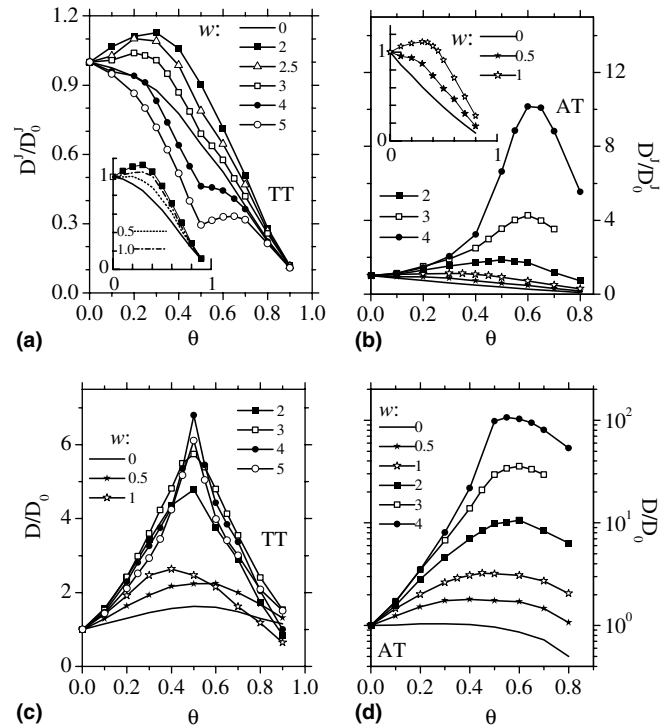


Fig. 8. Jump (a and b) and collective (c and d) diffusion coefficient for repulsive particles on heterogeneous chains with  $\Delta E = 2$  for TT and AT jumping mechanism, respectively.

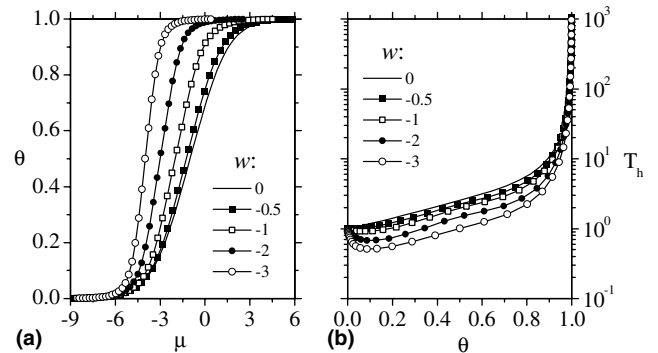


Fig. 9. Effect of attractive interactions on adsorption isotherms (a) and thermodynamic factors (b), for heterogeneous chains with  $\Delta E = 2$ .

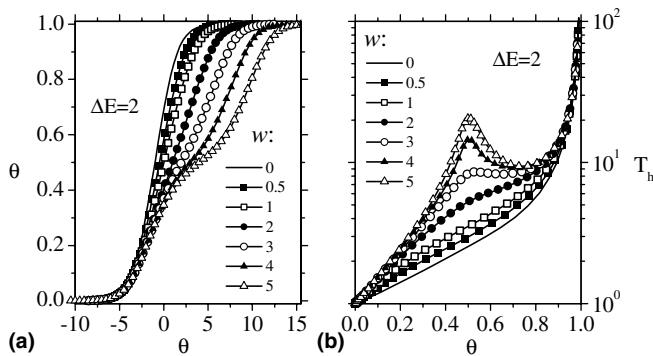


Fig. 7. Effect of repulsive interactions on adsorption isotherms (a) and thermodynamic factors (b), for heterogeneous chains with  $\Delta E = 2$ .

(to the right or to the left) becomes less probable because both the final and initial states are determining the transition rate, and  $D^J$  becomes strongly depressed showing a minimum, more pronounced for stronger repulsive interactions. On the contrary, for the AT mechanism, where the transition rate depends only on the initial state, jumps to a site with an occupied NN are not depressed and jumps away from a site with an occupied NN are enhanced by repulsive interactions, this results in a strong increase of  $D^J$  near half coverage, the stronger the larger repulsive interactions, showing a broad maximum. By combining the behaviors of the thermodynamic factor and the jump diffusion coefficient, the behavior of the collective diffusion coefficient is readily obtained.

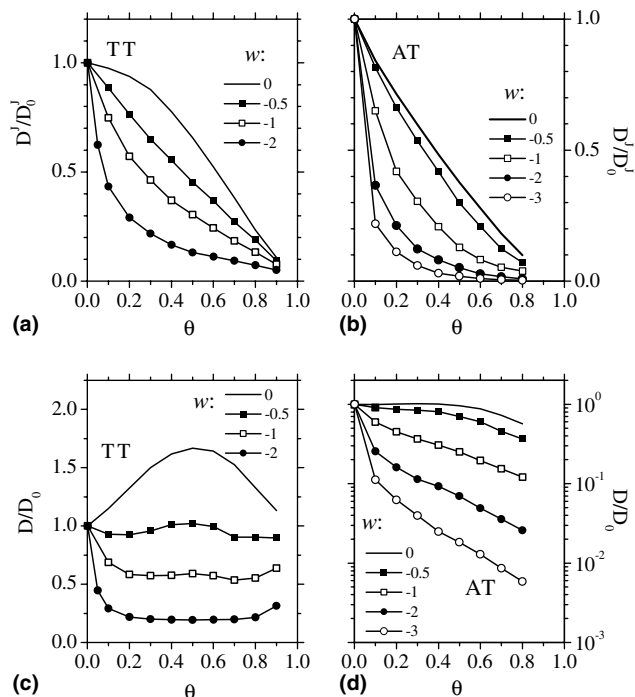


Fig. 10. Jump (a and b) and collective (c and d) diffusion coefficient for attractive particles on heterogeneous chains with  $\Delta E = 2$  for TT and AT jumping mechanism, respectively.

#### 4. Conclusions

The diffusion of adsorbed particles in one-dimensional heterogeneous lattices has been studied through Monte Carlo simulation. Heterogeneity has been introduced by considering a bivariate ordered chain of alternating patches of size  $l$  of deep and shallow adsorbing sites, whose difference in adsorption energy defines the heterogeneity strength,  $\Delta E$ . Ad-particles may interact through a nearest-neighbor interaction energy,  $w$ . Simulations are tested against exact solutions obtained for the case of a homogeneous chain, showing an accurate agreement. Adsorption isotherms, thermodynamic factors and the jump and collective diffusion coefficients are obtained showing the separate effects of lateral interactions for homogeneous lattices, of heterogeneity for non-interacting particles, and the combined effects of heterogeneity and interactions. In all cases the diffusion coefficients turned out to be highly sensitive to the parameters. In addition, two jumping mechanisms have been considered, the TT and the AT mechanisms, leading to qualitatively different behaviors in the diffusion coefficients. In particular, the collective diffusion coefficient, as a function of coverage, a measurable quantity, is found to be nearly symmetric around half coverage for the TT mechanism, while for the AT mechanism it is not, a feature that may give information about the jumping mechanism from the analysis of experimental data. The kind of study presented here may be helpful

in analyzing experimental data about diffusion of ad-atoms in low dimensionality systems, as, for example, in the systems studied experimentally in Refs. [27–30].

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