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Subdiffusive Behavior in Crowded Environments: Impact of Obstacle Mobility and Spatial Restrictions

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Abstract: Biological systems are generally dense reaction-diffusion systems. Therefore, determining the mechanism of motion in such systems is of crucial importance in understanding their dynamics. Subdiffusive behavior is very common in biological systems but its origin usually does not have a clear explanation. One attempt to explain this behavior is the presence of randomly placed stationary obstacles in a medium filled with molecules of a certain medium. With an appropriate concentration of obstacles, the molecules of the medium cease to perform classic Brownian motions and motion becomes subdiffusive. This mechanism seems to be well documented in both simulations and experiments. The question arises whether a similar effect can be obtained in systems where obstacles are not stationary, but their mobility is drastically reduced comparing to medium molecules, or the reduction in mobility is combined with a limitation in movement (the movement of obstacles resembles, for example, the Orestein-Ulhenbeck movement). Is it possible to observe subdiffusion behavior in such a situation? We try to answer this question on the basis of Monte Carlo simulations based on the Dynamic Lattice Liquid (DLL) model. Based on the concept of cooperative movements, this model has a unique feature that allows one to take into account the correlation of movements between the elements that make up the examined system, which is important in the case of high densities due to the strict correlation of movements between the moving elements. The tests concern systems where obstacles were single beads whose mobility was changed with additional restrictions imposed on the displacement. It was shown that no entrapment of medium molecules was observed and a slight deviation from normal diffusion was also shown.

Key words: anomalous diffusion, lattice model, macromolecular crowding, Monte Carlo method

I. Introduction

A subdiffusive behavior can be explained theoretically using three widely accepted scenarios. The first one, considered to be the simplest, is "fractional Brownian motion", which consists of generalizing Brownian motions, where we apply random changes of positions that are not independent as in classic Brownian motions but show long-term correlations [1–5]. The second frequently used scenario is the so-called "continuous-time random walk" (CTRW) based on power distribution of waiting times for movement [6–10]. The third scenario is the only one that provides a clear picture of the appearance of subdiffusive behavior in a system. In this model, it is assumed that a certain part of the system is filled with randomly placed stationary objects of various sizes and shapes called obstacles and elements of the

medium move between them [11–15]. The basic quantity commonly used in the description of dynamics in this type of systems is the mean square of the displacement (MSD), which is defined as follows:

$$\left\langle \Delta r^2 \left(t\right) \right\rangle = \frac{1}{n} \sum_{i=1}^{n} \left[\boldsymbol{r_i} \left(t\right) - \boldsymbol{r_i} \left(0\right) \right]^2 , \tag{1}$$

where $\boldsymbol{r_i}\left(t\right)$ is a vector describing the position of the ith element after time t relative to the initial position $\boldsymbol{r_i}\left(0\right)$. Using the Einstein's relation, the diffusion coefficient D can be determined as follows:

$$\left\langle \Delta r^2 \left(t\right) \right\rangle = 4Dt, \;\; t \to \infty. \tag{2}$$

The formula (2) is valid for normal (Fickian) diffusion, i.e., when the MSD depends linearly on time. In systems with anomalous diffusion, the dependency of the MSD on time has the form:

$$\left\langle \Delta r^2 \right\rangle \sim t^{\alpha}, \tag{3}$$

with the exponent $\alpha \neq 1$. Subdiffusive motion corresponds to values of α lower than 1. According to the theory, e.g., on a triangular lattice, where obstacles correspond to single lattice nodes, the percolation threshold is 0.5, i.e., half of the nodes are occupied by obstacles, and the exponent α takes the value 0.659 [11]. One should remember that the theoretical values like the exponent α are not universal because, first of all, the location of the percolation threshold strongly depends on the size of the obstacles [16, 17]. Secondly, correlation (or lack of it) plays an important role in the movement of the studied elements [18]. Recently, two systems based on a triangular lattice with fixed matrix of impenetrable obstacles were examined and compared [19]. In the first one a single element moved between obstacles and did not interact with other elements. In such a case, the dynamic percolation threshold, i.e., the threshold at which the movement becomes restricted, coincides exactly with the percolation threshold resulting from the theory. Moreover, the exponent α also shows a good agreement with the theory. The situation changes dramatically when the movements of individual elements are correlated with each other, as is the case of real dense systems occurring in the nature. In this case, the Dynamic Lattice Liquid (DLL) algorithm based on the concept of cooperative movements, taking into account the strict correlation between the movements of molecules in the liquid, indicates the dynamic percolation point corresponding to the concentration of obstacles close to 0.38 and the exponent $\alpha \approx 0.38$. Such a low value of the exponent α is not surprising because such values are obtained in real experiments [20, 21].

The assumption of immobility of obstacles is very convenient from the point of view of simulation practice; however, a question arises what the diffusion will look like in a system where the obstacles are not stationary and we let them move slightly. Also, what happens if the movement of obstacles is spatially constrained? A partial answer to this question was recently given and it was confirmed that these mobile obstacles lead to the temporary subdifussive behavior only [19]. In the present work, we study the diffusion in a system in which the obstacles correspond to single nodes of the lattice, whose mobility is limited. Additionally, a condition limiting their movement is imposed on them – the movement of obstacles resembles the Orestein-Ulhenbeck movement [22]. We performed Monte Carlo simulations employing the aforementioned DLL model.

II. The Models and the Simulation Methods

The application of the DLL model and simulation method in the case of a crowded environment was described in detail in [23] and therefore we give only a brief description here. The DLL model fulfills the continuity equation and provides the correlated movements of molecules as in a real liquid. Moreover, dynamic properties, which it produced, were in good agreement with those established experimentally and theoretically for liquids [24, 25]. The simulation is performed at the highest possible density, which cannot be obtained using other simulation methods: Molecular Dynamics studies of models with a matrix of immobilized obstacles were usually performed at the concentration up to 0.6 [14, 26, 27]. The DLL model is basing on the concept of strictly cooperative motion of molecules in dense systems. In this model, molecule vibrate near quasi-localized points (remaining at a given place) sometimes being involved in a motion correlated with their neighbors, which results in their translations [24–26]. This picture of a motion in a molecular liquid is commonly accepted and consistent with a picture obtained by Molecular Dynamics simulations of dense hard disks and Lennard-Jones systems [28, 29]. The model was coarse-grained where identical beads represented medium molecules or obstacles. The positions of the objects were limited to vertices of a triangular lattice and all lattice sites in the system were occupied by beads. Objects do not exhibit any simple translational motion because all neighboring lattice sites are occupied. But the DLL model allowed determining the conditions required for collective molecular translations. Each displacement of an object from its position is considered as an attempt of a movement to a neighboring lattice site along lattice vectors.

Cooperative rearrangements in the DLL model on the lattice have a form of closed loops of displacements (Fig. 1). Objects that did not belong to a closed loop consisting of at least three objects were immobilized at a given time step. An element chosen randomly as an immobile obstacle cannot take place in a cooperative loop during the entire simulation run. A time unit corresponds to an attempt to change positions of all objects in the system simultaneously. The simulation scheme of the DLL algorithm presented in Fig. 1 is the following:

1. A random vector field of motion attempts with a vector assigned to each bead and pointed towards one of the nearest-neighboring lattice sites was generated.
2. Groups of vectors coinciding with contours of closed continuous paths (loops), showing ways of possible cooperative rearrangements were selected.

3. Objects (beads) belonging to these closed paths (loops) were rearranged along these paths by shifting them to the neighboring sites. It should be underlined that the algorithm based on the above assumptions was strictly parallel.

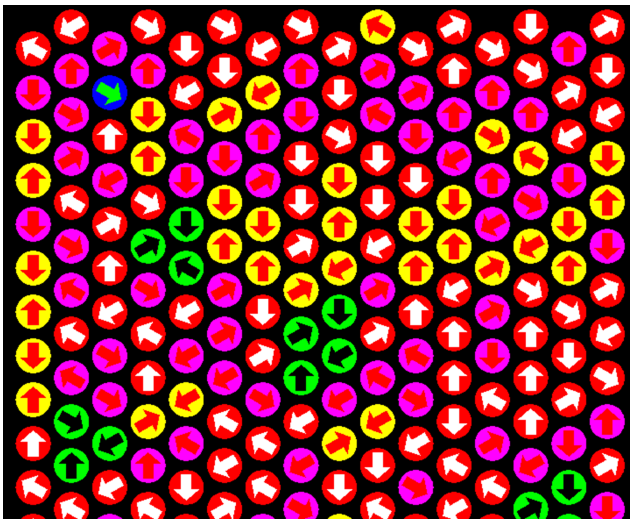

Fig. 1. Illustration of a vector field representing attempts of molecular displacements towards neighboring lattice sites as assumed in the DLL model. The marked areas represent various local situations: (1) elements (yellow) try to move in the opposite direction (unsuccessful attempts), (2) an attempt of motion starts from an element (violet) so that, when moved, it would not be replaced by any of its neighbors (unsuccessful attempts), and (3) each green element replaces one of its neighbors (successful attempts)

The simulations were carried out in the simulation box $L \times L$ where $L = 256$ with periodic boundary conditions employed along the x and y axes. It was previously shown that if the system is larger than 64×64, the statistic of cooperative loops of displacement does not depend on the size of the Monte Carlo box [24]. A single simulation trajectory consisted usually of ca. 10^8 Monte Carlo simulation steps. The simulations were repeated at least 10 times and each simulation run was performed for different random matrices of obstacles (about 30 different matrices). The results were averaged over all runs for a given set of input parameters. The concentration of obstacles (each having a size of a lattice node) was defined as the ratio of the sites occupied by obstacles to the total number of lattice sites in the system: $c = N/L^2$, where N is the number of obstacles in the system.

There were three types of obstacles considered in this work:

1. Stationary obstacles that correspond to disabled elements in a network node, i.e., these elements are immobilized.
2. Obstacles that move with reduced mobility. This reduction was imposed as a probability of motion of an element and was varied between 1 (obstacles were as mobile as medium molecules) and 10^{-5} (obstacles were 5 orders of magnitude slower than medium molecules).
3. Obstacles that move with reduced mobility (the same reductions as given above) and at the same time their motion was limited in space. These obstacles were allowed to move by one or two lattice nodes (to neighbors or to the second neighbor on the lattice).

III. Results and Discussion

The main factors that affect the type of transport in the system are the topology of the system and the conditions in which the transport takes place. Therefore, it is very important whether we take into account the obvious fact that in dense systems such as liquids the movement of elements is closely correlated or not. In our case, the movement of elements in all cases is closely correlated due to the conditions imposed by the DLL algorithm. Before proceeding to the description and discussion of the movement of the medium elements, let us focus on the different variants of the movement of obstacles. Fig. 2 presents a comparison of the movement of obstacles when their mobility has been drastically limited and additional restrictions have been imposed on their spatial movement. It is worth noting that the motion of slowed-down obstacles (black lines) has a Brownian character in the considered time interval. The movement of obstacles with additional spatial constraints (blue and red lines) largely retains the character of slow-moving obstacles, then tends to a constant value, which is related to the location of the movement.

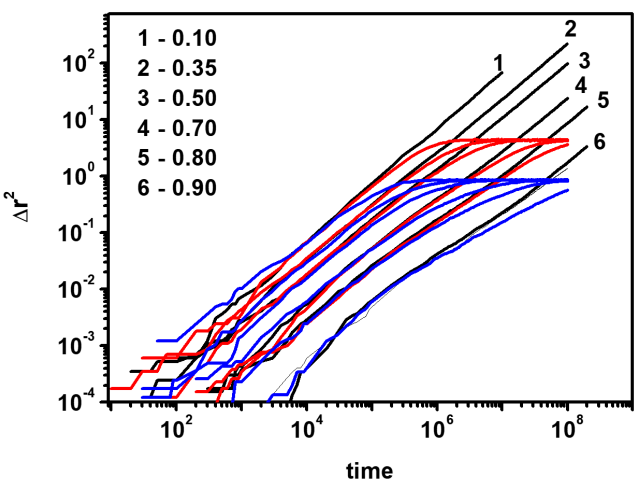

Fig. 2. MSD of molecules in the system with obstacles whose mobility has been reduced 10^4 times. The black color corresponds to the system where the spatial movement of obstacles has not been restricted. The red color corresponds to the system where the movement of obstacles has been restricted to two lattice constants. The blue color corresponds to the system where the movement has been restricted to one lattice constant. The concentration of obstacles is given in the inset

The motion of two-dimensional liquid molecules with close correlation of moving elements in the presence of stationary obstacles was presented in [18]. It was found that the dynamic percolation threshold appears at a concentration of obstacles $c = 0.38$ where the obstacles were single

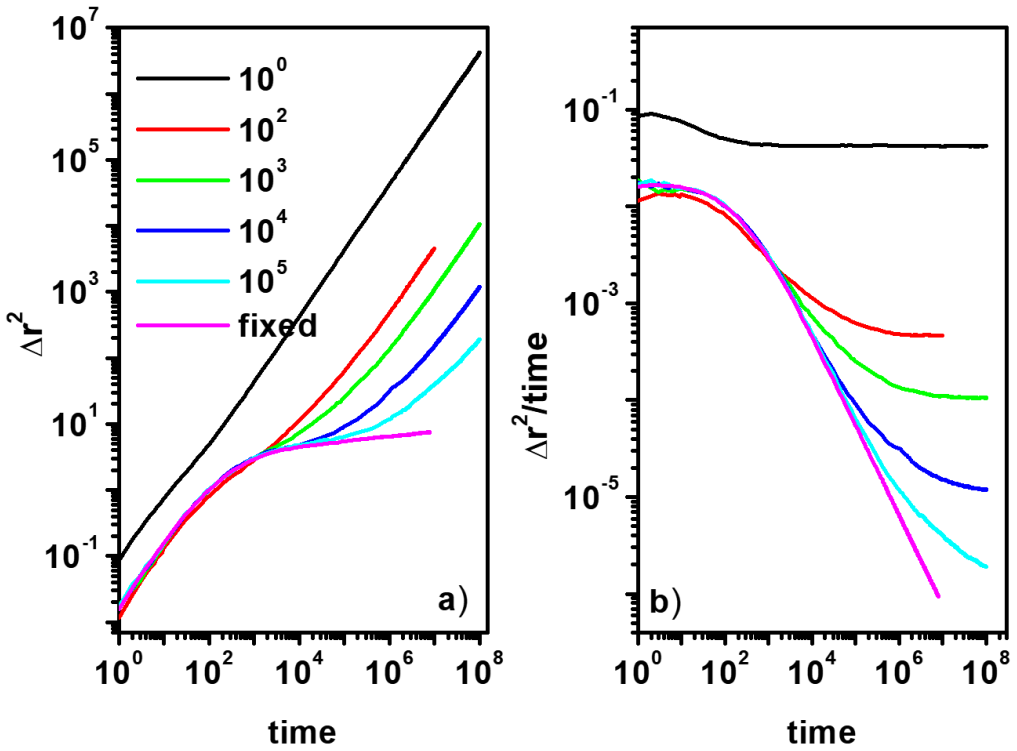

Fig. 3. MSD (a) and MSD/time (b) for molecules of the medium for the concentration of obstacles $c = 0.5$. The case of obstacles with the mobility reduced 10^1–10^5 times and spatially limited to one lattice constant compared to the case where the obstacles are fixed

beads immobilized in lattice nodes. Fig. 3a shows MSD of liquid molecules for different mobility of obstacles (the mobility varies from full mobility to the reduced one by the factor 10^5; additionally, results for systems with obstacles that are completely immobilized are included into this figure) with the concentration of obstacles $c = 0.5$. A spatial constraint was imposed on movable obstacles that they can move randomly according to the conditions of the DLL algorithm for a distance of one lattice constant relative to the initial position. This concentration of obstacles corresponds to the percolation threshold of beads on a triangular lattice, which is considerably higher than the concentration corresponding to the dynamic percolation (0.38) obtained as a result of simulations employing the DLL algorithm [11, 18]. Therefore, in a system with stationary obstacles above this threshold, the flow is completely blocked and the movement of the medium molecules is localized and limited to a small area. The curve that corresponds to the situation where we consider obstacles with additional spatial constraints for which mobility has not been reduced, is very similar to the case where obstacles are not present at all. The curves that describe MSD in the case of limiting mobility from 10^0 to 10^5 times show a similar character, i.e., we can distinguish three short regions in which we observe a Brownian motion corresponding to local motion. One can also see regions where the diffusion slows down and regions where the diffusion (over a long period of time) exhibit an apparent tendency to return to the Brownian diffusion. The MSD/t curves presented in Fig. 3b allow a better capture of these regions.

The image presented above, obtained on the basis of the MSD analysis, can be confirmed by the behavior of the position correlation function which we define as follows:

$$\rho(t) = \frac{1}{n}\sum_{i=1}^{n} m_i(0) m_i(t), \tag{4}$$

where $m_i(0) = 1$ and $m_i(t) = 1$ or 0, depending whether or not the i^{th} bead occupied its original position (at $t = 0$) and at a given time t, respectively.

In Fig. 4 we present the position correlation function of the molecules of the medium for the concentration of obstacles $c = 0.5$. Here, one can distinguish three regions of behavior: the first, in which the value of the correlation function decreases relatively quickly, the second, during which the arrested elements of the medium wait for the possibility of movement, and the third, in which the correlation function disappears completely. Some controversy may arise from the fact that we observe such a big difference in the movement in the first region between the variant where the mobility of obstacles was not reduced and the situation where the mobility of obstacles was reduced 10^2 times or more. Moreover, these curves are very similar in the initial region and there is no clear difference between them and the curve describing the behavior for stationary obstacles. One can easily explain this behavior taking into consideration the assumptions of the DLL algorithm. The probability of taking part in a cooperative loop in a system without obstacles is about 0.09, which corresponds to an average of one movement of any element in about 11 time steps. If we reduce the mobility of

an element (in our case, obstacles which move without constraints) 10^2 times or more they are locally almost immobile. Therefore, an appropriate time has to elapse, and this time corresponds to the diffusion slowdown.

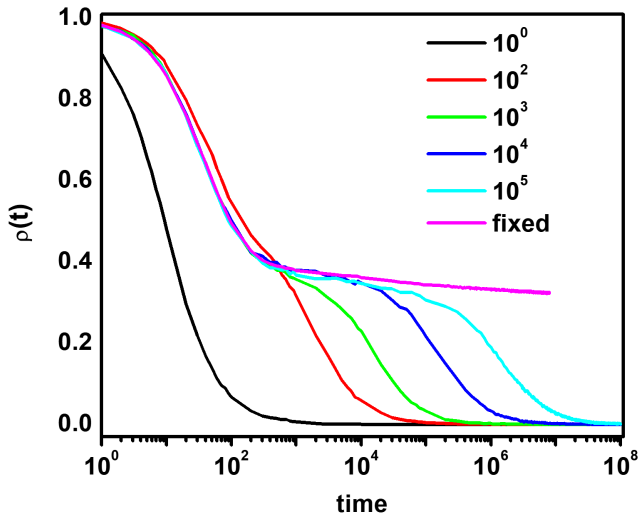

Fig. 4. A comparison of the position correlation function of the molecules of the medium for the concentration of obstacles $c = = 0.5$. The case of obstacles with the mobility reduced 10^1–10^5 times and spatially limited to one lattice constant compared to the case where the obstacles are fixed

In order to fully analyze the impact of a slow movement of obstacles on the behavior of the medium's elements, let us consider a situation in which the mobility of obstacles is drastically limited by the factor 10^5 along with a simultaneous spatial limitation as in the case considered previously, i.e., an obstacle can randomly move a distance of one lattice constant (relative to their initial position). This procedure is due to the fact that the observed effects are very subtle and reveal themselves in situations of drastic parameter limitations. Moreover, a very long observation time is required here. Fig. 5a shows a comparison of the MSD of the medium elements when the obstacles are stationary and the movement of the obstacles has been restricted as described above.

When the concentration of obstacles does not exceed 0.3, we observe similar behavior in both cases. The situation starts to change after exceeding this concentration of what can be related to the fact that we are approaching the dynamic percolation threshold, which in the case of the DLL model is 0.38. For the concentration $c = 0.38$, there is a clear difference between both cases. The time of staying in the diffusion slowing-down region increases dramatically. While in the case of stationary obstacles we observe a subdiffusive motion, in the case of moving obstacles diffusion remains normal for a long time of observation. The transition to the anomalous diffusion seems to be observed for higher concentrations of moving traps above the concentration 0.7, which is clearly shown in Fig. 5a. A weak subdiffu-

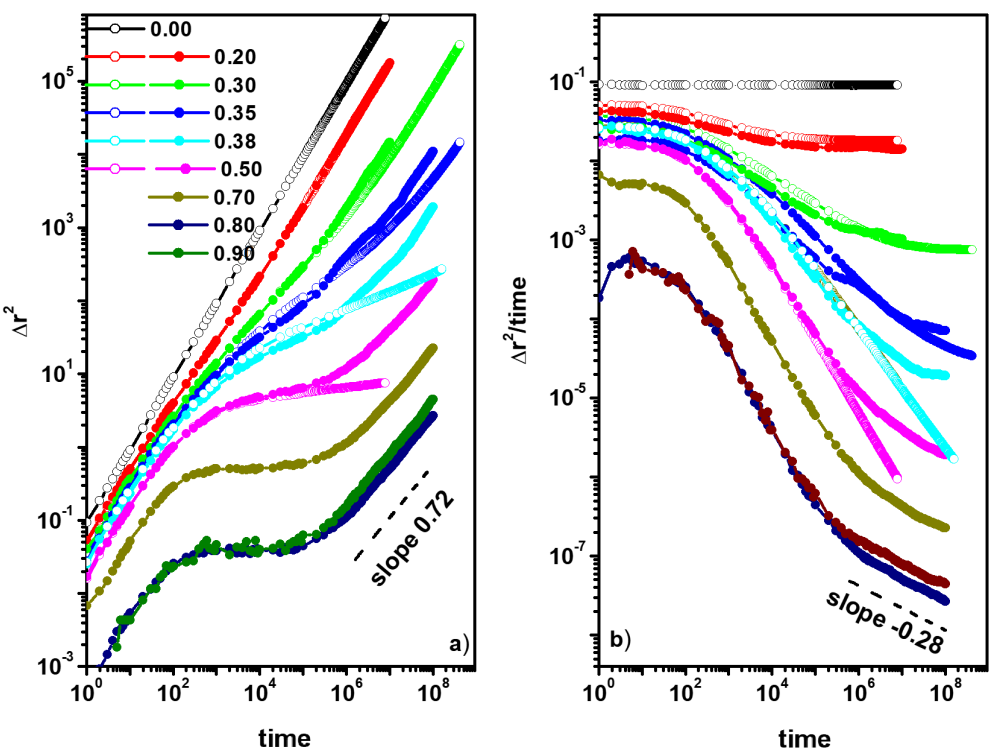

Fig. 5. MSD (a) and MSD/time (b) for molecules of the medium. The case where the mobility of obstacles has been reduced 10^5 times and spatially limited to one lattice constant network (solid symbols) and the case where obstacles are immobile (open symbols). The concentrations of obstacles are given in the inset

sive behavior seems to be clearly visible for concentrations of moving traps 0.8 and 0.9 which is much more than obtained within the frame of the DLL model (0.38) or given by the theory (0.5). Moreover, the exponent α for these cases is close to 0.72, which exceeds the exponent α for the DLL model with immobile obstacles (between 0.37 and 0.38) or predicted in the classic case of stationary obstacles (0.659). The MSD/t curves presented in Fig. 5b allow a better capture of the regions.

From the above considerations, one can conclude that the subdiffusive effect that we observe is very subtle. In order to determine the actual state of affairs, let us use the so-called non-gaussian parameter $\alpha_2(t)$. It is a sensitive quantity which allows one to recognize the character of the motion and it is defined as [30, 31]:

$$\alpha_2(t) = \frac{\langle \Delta r^4(t) \rangle}{2\langle \Delta r^2(t) \rangle^2} - 1. \tag{5}$$

This parameter takes values close to zero in the case of normal (Fickian) diffusion and becomes significantly greater than zero in the case of anomalous diffusion.

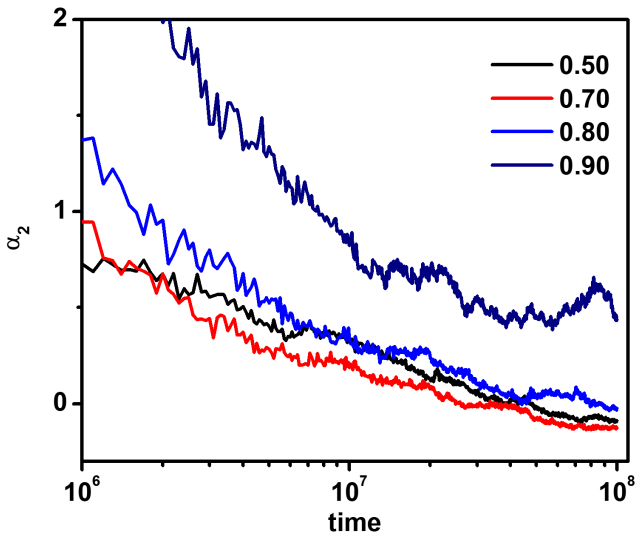

Fig. 6. The non-gaussian parameter $\alpha_2(t)$ for long observation times. The case of mobile obstacles with mobility reduced 10^5 times. The concentrations of obstacles are given in the inset

Fig. 6 shows $\alpha_2(t)$ for long observation times in the case of moving obstacles (mobility reduced 10^5 times) and for some concentrations between 0.5 and 0.9. The presented results indicate that the curves corresponding to concentrations of 0.5–0.7 for long observation times show the tendency to return to the normal diffusion. Only the curve corresponding to the concentration 0.9 shows values clearly greater than zero (although these values are not too large) with a tendency to stabilize. The results obtained from studies of the position correlation function indicate that in systems with even very low mobility of obstacles and even at high values of their concentration we do not observe the phenomenon of entrapment of medium molecules.

Fig. 7 shows a comparison of the position correlation function for the case of stationary and moving obstacles, which was considered above, i.e., the mobility of obstacles is reduced 10^5 times with simultaneous spatial limitation to one lattice constant. In all cases, there is a clear tendency towards complete relaxation.

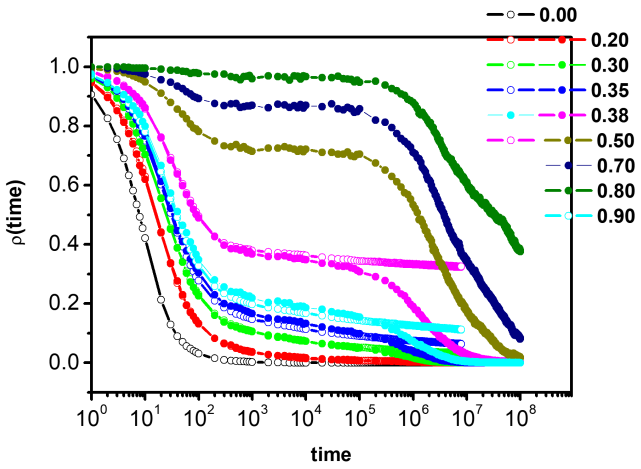

Fig. 7. The position correlation function. The case of fixed obstacles (open symbols) and mobile obstacles with mobility reduced 10^5 times (solid symbols). The concentrations of obstacles are given in the inset

Taking into account the presented results, it can be concluded that in the case of moving obstacles, even by introducing drastic restrictions on their mobility and spatial displacement restrictions, we can observe no signs of entrapment of medium molecules with a slight deviation from normal diffusion but this effect is generally weak. In the case of limiting the mobility of obstacles with the simultaneous introduction of restrictions on their spatial movement, the main factors generating the dynamics of the system are the concentration of obstacles, their mobility, their position relaxation time, i.e., the time after which the obstacle returns to its initial position.

Finally, systems with different concentrations of obstacles were compared, in which the mobility of obstacles was significantly reduced (10^4 times) but no spatial restrictions were introduced. The mobility was limited in the same way as mentioned above, and the spatial restriction allows for random movement around the starting point no more than two lattice constants (longer relaxation time than when the obstacle oscillates only over a distance of one constant). The results are presented in Fig. 8a and MSD/t curves are shown in Fig. 8b for a better capture of regions of normal and sudiffusive diffusion. The obtained results indicate that in all cases, on a time scale corresponding to times shorter than the time after which the molecules of the medium leave the region of the diffusion slowdown, the elements move in the same way, regardless of the imposed conditions. After exiting the diffusion slowdown region, differences in behavior can be noticed depending on the case under consideration. And so, for the variant in which no spatial constraints have been imposed, we observe a return to Fickian diffu-

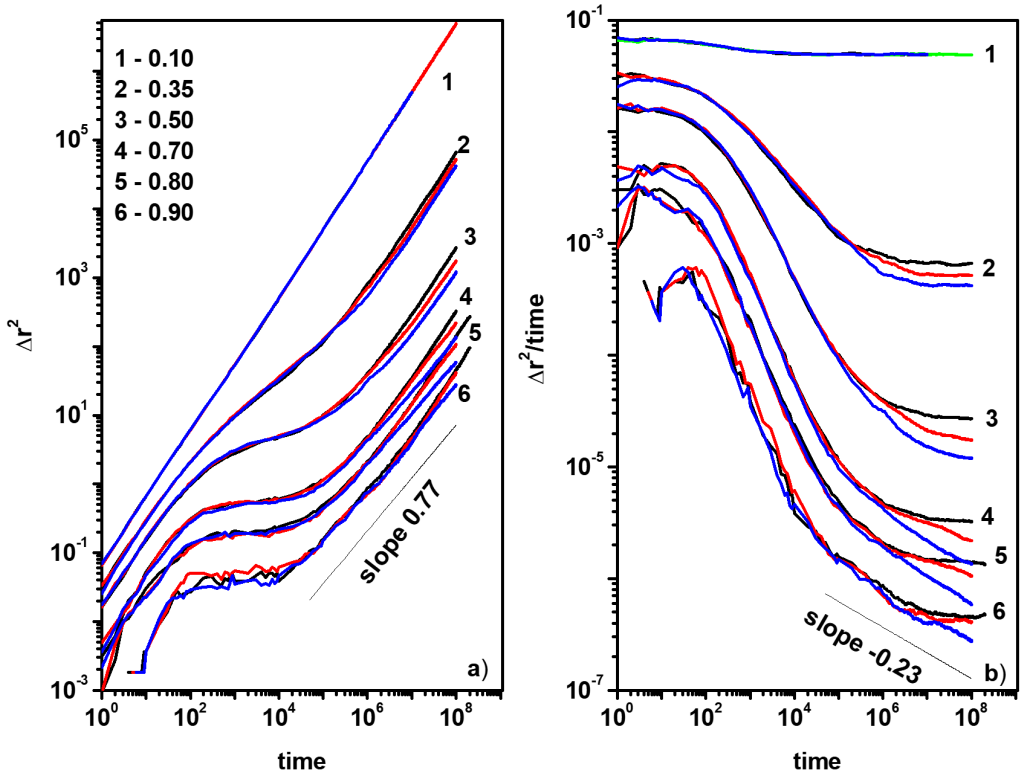

Fig. 8. MSD (a) and MSD/time (b) for molecules of the medium where their mobility has been reduced 10^4 times. The case of obstacles spatially limited to one (blue) and two (red) lattice constant and the case of obstacles with no spatial limitation (black). The concentrations of obstacles are given in the inset

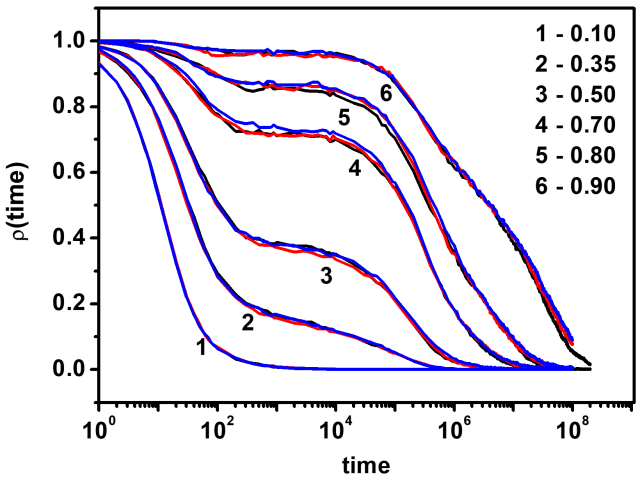

Fig. 9. Position correlation function for molecules of the medium where their mobility has been reduced 10^4 times. The case of obstacles spatially limited to one (blue) and two (red) lattice constant and the case of obstacles with no spatial limitation (black). The concentrations of obstacles are given in the inset

sion (black curves parallel to the time axis are clearly visible). In the case when the spatial constraint is two lattice constants, a certain deviation is visible after a long observation time, especially for the high concentrations of obstacles. The strongest effect can be observed in the third case, i.e., where obstacles can be moved by one lattice constant only. In this case, with the increase in the concentration of obstacles after exceeding the concentration corresponding to the percolation threshold (determined for the DLL model), we observe an increasingly clear deviation from a normal diffusion behavior. For long times and high concentrations, the exponent α is close to 0.77, which is slightly more than in the case considered in Fig. 5. It has to be stressed, however, that the nature of these differences is very subtle and requires a very long observation time.

The fact that the differences in cases where obstacles with very limited mobility are additionally imposed with spatial constraints are very subtle is confirmed by the behavior of the position relaxation function shown in Fig. 9. It can be observed that regardless of the considered variant or concentration of obstacles, the curves describing the position relaxation functions are practically indistinguishable.

IV. Conclusions

Computer simulations of a motion of liquid molecules in crowded environments in two-dimensions were carried out. The Dynamic Lattice Liquid model was used for these simulations because of its ability to work at high densities employing cooperative motion objects in the system. The model was coarse-grained, molecules were placed in a triangular

lattice, and the system was athermal. We studied the following models of crowded environments: immobilized obstacles, mobile obstacles and mobile obstacles with their motion considerably confined (all obstacles were of the size of solvent molecules). The influence of the molecular transport and the analysis of critical parameters in most of these systems were already carried out and therefore we have tried to compare the diffusion processes in such systems looking for the conditions of appearance of anomalous diffusion.

The dynamics of liquid molecules and obstacles was studied by the analysis of mean-square displacement and position autocorrelation function. In the case of immobile obstacles transient subdiffusive motion appears but finally a normal diffusion is recovered. But when the concentration of obstacles exceeds the percolation threshold the motion becomes limited. If obstacles are allowed to move, considerably slower than the molecules of medium, even a few orders of magnitude, subdiffusion occurs, but then normal diffusion is restored and the anomalous diffusion was transient in all cases. The slower the obstacles, the longer the subdiffusion region lasts. The confinement of mobile obstacles, i.e., imposing a spatial restriction on their movement does not change much in the picture of the dynamics of the studied systems. However, it should be noted that for high mobility constraints (probability of movement reduced by 10^4–10^5 times) and high concentrations of obstacles (above 0.70) with the spatial constraint, a weak subdiffusive behavior is observed, where the exponent $\alpha < 0.78$. Moreover, as obstacle mobility decreases, this exponent decreases slightly. This suggests that more pronounced subdiffusive behavior is to be expected with even lowered mobility. The above results can be relevant for studies of diffusion in biological systems where heterogenous media commonly occur and affect biological functions, e.g., in cells or lipid membranes. To get a better description of these processes more realistic models which take into account interactions and chemical reactions have to be developed.

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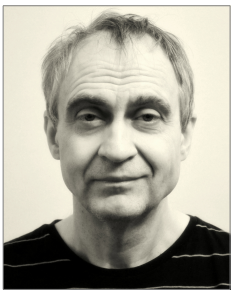

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