RAPID COMMUNICATION

Collective transport of Lennard–Jones particles through one-dimensional periodic potentials*

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The surrounding media in which transport occurs contains various kinds of fields, such as particle potentials and external potentials. One of the important questions is how elements work and how position and momentum are redistributed in the diffusion under these conditions. For enriching Fick's law, ordinary non-equilibrium statistical physics can be used to understand the complex process. This study attempts to discuss particle transport in the one-dimensional channel under external potential fields. Two kinds of potentials—the potential well and barrier—which do not change the potential in total, are built during the diffusion process. There are quite distinct phenomena because of the different one-dimensional periodic potentials. By the combination of a Monte Carlo method and molecular dynamics, we meticulously explore why an external potential field impacts transport by the subsection and statistical method. Besides, one piece of evidence of the Maxwell velocity distribution is confirmed under the assumption of local equilibrium. The simple model is based on the key concept that relates the flux to sectional statistics of position and momentum and could be referenced in similar transport problems.

Keywords: transport, external potential, collective diffusion, Maxwell velocity distribution

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1. Introduction

There are three laws of transport in nature. The first law is Fourier's law, which describes how heat diffuses in a medium, while the second is Ohm's law. The third transport law, i.e., Fick's first law, successfully explains the clear relationship between particle flux and concentration. If a transitory perturbation is induced, a relaxation process will revert the system back to the equilibrium state within the relaxation time. If a ceaseless force is applied, the transport phenomenon occurs because of the ceaseless flux. In contrast to other deterministic analytical descriptions, Fick's law involves the statistics related to the second law of thermodynamics. What drives particles to transport? It is not that particles themselves push each other to move, because each particle is independent, but only the probability.[1] Knowledge of transport phenomena through statistics might describe social phenomena in nontraditional physics applications.[2] Thus, diffusion is in the field of statistics. A system tends to come back to an equilibrium state when it is in a non-equilibrium state, and balances the entire distribution for more harmony.

The equilibrium adsorption and surface properties of the Lennard–Jones particle in one-[3] or two-dimensional[4,5] pores have been successfully predicted using a weighted density functional theory or molecular simulations. Next, we focus on the statistical physics of non-equilibrium states. In biology, equilibrium equals the death of the life, and non-equilibrium is very usual in the creature; the essence of chemistry process is non-equilibrium, because of no macroscopic chemistry in equilibrium. Nevertheless, solving problems involving the non-equilibrium state is so complex that one still needs to depend on experiments, the essential element provided by the development of the modern computer.

Let us disregard the fact that a particle is more or less affected by realistic forces, and then so many research studies based on Fick's law without any force spring up firstly. Liu *et al.* obtained the Fick diffusion coefficients in the liquid mixtures of equilibrium states.[6] Chvoj has investigated diffusion transformations depending on the temperature.[7] Furthermore, the diffusion issues mixed with external forces are becoming the hot points. Prinsen and Odijk calculated some of the parameters such as the collective diffusion coefficients of proteins, considering the interaction of electrostatic and adhesive forces.[8] Yu *et al.*[9] and Zhong *et al.*[10] also did similar work for the collective diffusion. Tarasenko discussed the collective diffusion in a one-dimensional homogeneous lattice.[11]

However, the constrained motion is ubiquitous in the models for more intricate systems. Siems and Nielaba studied the diffusion and transport of Brownian motion in a two-dimensional microchannel, combining periodic potentials and

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forces.[12] Given biological or soft condensed matter scenarios, both potential barriers and potential wells are of importance, as the external force is tangled in biological ionic channels, nanopores, and zeolites in materials science.[13] Ions in the channel are accelerated or decelerated by electric force arising from electric charges around the ion channel. In the two-dimensional tube, the shape of the tube affects the diffusion as well,[14] as the particles are accelerated or decelerated in the direction of propagation, by reduction or increase in degree of freedom in the width of tubes, let alone in the case of a deformable tube.[15]

In summary, diffusion coupled with the multifarious and composite forces, which is an interesting problem with practical applications, remains a challenge due to the major issue that the two fields of statistical physics that are reflected in stationary distributions, and molecular dynamics, which is reflected in particle transport, are difficult to combine.

Koumakis *et al.* used the run and tumble model to describe the kinetics of particles while traversing energy barriers.[16] Our work is a series of experiments conducted by computer with the method used being very similar to Wang, Yu and Gao's work, which studied the transport properties of Lennard–Jones (L–J) particles and their mixture.[17] We perform the simulation of particle transport in external potentials using Monte–Carlo method and molecular dynamics. More specifically, the particles with L–J potentials between one another move freely because of the concentration difference, as known from the Fick's law. There are also potential fields appended factitiously for the relationship that measures how the external potentials impact the diffusion coefficient.

This paper is organized as follows. Section 2 describes the model with schematic and some simulated elements, including external force field, internal particle potential, Metropolis and Verlet algorithm, and Fick's law. In Section 3, we deal with relevant parameters that need to be simplified. Simulation graphs in Section 4 show interesting results of gradual variations of the diffusion coefficients. Conclusions, applicability, and future prospects are discussed in Section 5.

2. Schematic and principles of the model

In particular, in the subcellular level, the electric field should be considered in mass transfer because the ions cannot pass through the channel smoothly because of the field effects arising from the charge. Static electric fields[18] and alternating current fields[19] in the surroundings can affect the diffusion coefficient in general. The diffusion becomes more complicated as the particles are affected by different forces in different locations. For example in biology, the transport phenomenon in the periodic tube is an ambiguous and intricate collective diffusion problem.[20] Meanwhile in the selectivity filter or protein channels,[21–23] the potential energy or the fields are particular to the external force fields, as ions transport through it.

Particularly in the ionic corrugated tube, particles are inevitably affected by the external force. Figure 1(a) displays the protomodel of observed biological ion channel. The equivalent one-dimensional model shown in Fig. 1(b) generalizes this in an abstract manner. In the schematic above, particles' transport from the left side of high concentration to the right side symbolizing low concentration is affected by the external alternating force. This implies that particles in the channel traverse through the external fluctuating potential field, but do not move up and down themself. The actual charges around the channel determine the potentials that affect the collective diffusion. When a positive ion is passing through the channel, if charges around the channel are negative, as shown in Fig. 1(c), the potential forms a well. Conversely, if they are positive, as shown in Fig. 1(d), the field forms a barrier. It is worthy of mentioning that the potential in this model does not change the potential of particles in total, but it does change the diffusion coefficient, in other words, the diffusion ability.

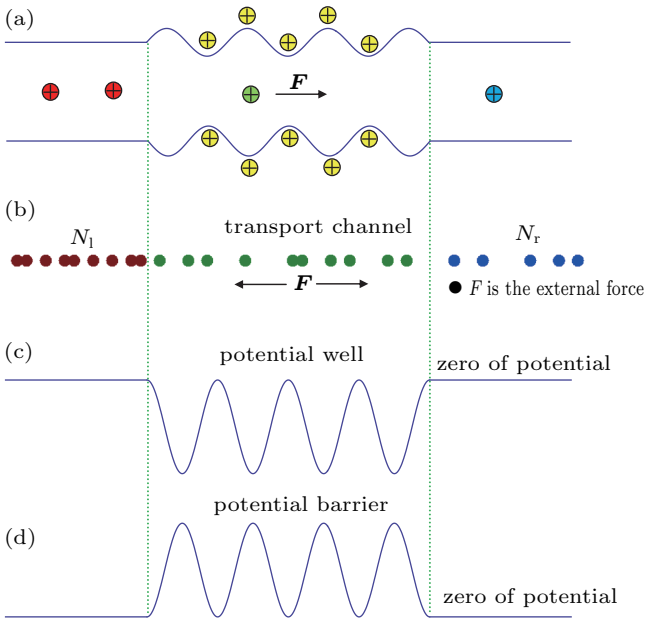


Fig. 1. (color online) In the biological ion channel (usually like a corrugated tube), ions are interacted inevitably by charges around the channel (a). This system is consistent with a channel, through which a particle is passing in an external potential field (b). Usually, if the charge is an electron, the external potential can be considered as a potential well (c). On the contrary, if positive, the potential field is a potential barrier (d). The two ends of the channel are the particle reservoirs which maintain the concentration of the ions.

Finite size effect is a normal phenomenon typical to many physical systems, such as thermal and electrical systems.[24,25] Therefore, the one-dimensional model can be used effectively. In this model, as shown in Fig. 1, there are two particle reservoirs on the left and the right side separately. Between these particle reservoirs, there is a one-dimensional channel for particles being transported between reservoirs back and forth. Therein, the fixed boundaries are rooted in the left and

right extremes of the system. With the help of the Monte–Carlo method, the particle number in the two reservoirs can be maintained at a steady value. The particle–particle interaction is described according to the Lennard–Jones potential. The Langevin random heat baths[26] regulate the temperature of the system and the velocity of each particle becomes a random variable that follows the Maxwellian distribution. The molecular dynamics and Verlet algorithm can predict all kinetic parameters. The program sets 0.55 fs as the time step. As shown, for the particles transporting under the one-dimensional external potential, potentials with multifarious parameters are applied to this channel, which influence the diffusion while the particles move freely.

When the transport procedure occurs, every particle in the channel experiences the external force from the potential. To present the situation in a general manner, not only simple trigonometric functions of potentials but potential wells and barriers are introduced in the calculation. To reflect two inverse conditions, the potential well makes the particles drop into the field in the channel, and the barrier impedes particles from moving into the channel. The external potential is defined as $U_{\rm w}$ and $U_{\rm b}$ for the potential wells and barriers respectively. The mathematical form is

$$\begin{aligned} U_{\rm w}(x) &= -F_0\frac{x_{\rm r}-x_{\rm l}}{2\pi n_{\rm p}}\left[1-\cos\frac{2\pi n_{\rm p}(x-x_{\rm l})}{x_{\rm r}-x_{\rm l}}\right] \\ &= -\frac{1}{2}U_0\left[1-\cos\frac{2\pi n_{\rm p}(x-x_{\rm l})}{x_{\rm r}-x_{\rm l}}\right], \end{aligned} \tag{1}$$

in which F_0 is the amplitude of the external force which is added factitiously; $n_{\rm p}$ is the period of that force; $x_{\rm r}$ and $x_{\rm l}$ are the coordinates of the right and left side respectively; U_0 is the depth or height of the potential. It obtains the exact potential value in the exact coordinate x. As the corresponding opposite field, the form of the potential barrier is the symmetry of the potential well

$$\begin{aligned} U_{\rm b}(x) &= F_0\frac{x_{\rm r}-x_{\rm l}}{2\pi n_{\rm p}}\left[1-\cos\frac{2\pi n_{\rm p}(x-x_{\rm l})}{x_{\rm r}-x_{\rm l}}\right] \\ &= \frac{1}{2}U_0\left[1-\cos\frac{2\pi n_{\rm p}(x-x_{\rm l})}{x_{\rm r}-x_{\rm l}}\right]. \end{aligned} \tag{2}$$

The metropolis algorithm, the most famous algorithm in the Monte–Carlo method,[27,28] is used to control the concentration in the particle reservoirs. Maintaining the chemical potentials in the end regions requires stochastic particle creation and deletion trials every 50 time steps, according to the grand canonical Monte Carlo (GCMC).[29] In the one-dimensional reservoirs, the two ends are the immobilized boundaries, and the particle amount in the reservoirs is set as N; however, the system is likely to create a particle if the amount is fewer than N. This probability of such creation is

$$P_{\rm cr} = \min\left[1, \exp\left(-\frac{\Delta U}{kT}\right)\right], \tag{3}$$

in which k is the Boltzmann's constant, T is the temperature of the particle reservoir, ΔU is the change in energy when a particle is added or created.

First, a random place of reservoirs would create a particle when the number of particles in the reservoir is less than N. If ΔU is under zero, however, the probability becomes 1, implying that the creation of a new particle is acceptable and the particle is given a new coordinate and a new velocity which obey Maxwell distribution. If ΔU is above zero, it must create another random number P between 0 and 1. Only when $P_{\rm cr} \geq P$, the newly created particle is acceptable and its coordinates and velocity are according to the probability of $\exp(-\Delta U/kT)$; otherwise, it becomes unacceptable and the new particle is deleted.[30]

Conversely, the system would probably delete a particle if the amount of particles is more than N. The probability is $P_{\rm dest} = \min\left[1, \exp\left(-\frac{\Delta U}{kT}\right)\right]$, and the operation is analogous to the situation, which previous works have discussed.[31,32]

While dealing with realistic problems, it is necessary to introduce interaction potentials in different kinds of material. The Lennard–Jones potential[33] is applied as the internal potential for particles in our simulated diffusion.

Using molecular dynamics[34] dynamic data such as displacement, velocity, and accelerated velocity data can be obtained. This analysis is performed using the modified Verlet algorithm.[29]

Moreover, the collective diffusion coefficient D is an important factor, based on the meaningful diffusion law, known as the Fick's law

$$\boldsymbol{j} = -D\frac{\partial c}{\partial L}, \tag{4}$$

in which D, the diffusion coefficient, represents the capacity of diffusion during the physical process and its unit is $\rm m^2/s$; $\boldsymbol{j}$ is the mass flux of the diffusion and its unit is $\rm mol/m^2{\cdot}s$; c is the concentration and the unit is $\rm mol/m^3$; L is the length of the channel.

3. Definition of relevant parameters

The parameters for Lennard–Jones potential are as follows $m = 1.67 \times 10^{-27}$ kg, $\sigma_0 = 0.258$ nm, and $\varepsilon_0 = 10.22$ K for the helium atom, and $k = 1.38 \times 10^{-23}$ J/K. All physical quantities in the simulation model need to be simplified: relative atomic mass m^* is the simplification of one hydrogen atom; the length is $L^* = L/\sigma_0$; the temperature is $T^* = T/\varepsilon_0$; the concentration is $c^* = c\sigma_0$; the potential parameters are $\varepsilon^* = \varepsilon/\varepsilon_0 = 1$ and $\sigma^* = \sigma/\sigma_0 = 1$; the average velocity is $\bar{\boldsymbol{v}}^* = \bar{\boldsymbol{v}}(m/\varepsilon_0 k)^{1/2}$; the potential is $U_0^* = U_0/\varepsilon_0 k$; the mass flux is $\boldsymbol{j}^* = \boldsymbol{j}\sigma_0(m/\varepsilon_0 k)^{1/2}$; and the collective diffusion coefficient is $D^* = D(m/\varepsilon_0 k)^{1/2}/\sigma_0$.

4. Results and discussion

In order to study the different conditions for mass transfer, various transport procedures under different situations such as the average concentration and differential concentration of reservoirs, the amplitude and cycles of the external force, the length of the channel and temperature of the system, were analyzed. Changing some conditions leads to similar diffusion trends irrespective of the potential wells or barriers; however, some changes lead to total disparate trends depending on the potential wells or barriers.

A few diagrams that show the relationship between diffusion coefficient and the various parameters have been provided. In the simulation, the default number of steps is 8×10^8, the temperature is 300 K, the channel length is 100 nm, and the periodic number of the potential field is 6, if there is no postscript.

Once the system stabilizes the flux, it will be in the stationary state. The non-equilibrium state is a special kind of stationary state. The particles reach a dynamic balance, which means that the system is in the minimum extreme value of the Hamiltonian,

$$H_N=\sum_{i=1}^{N}\left[\frac{\boldsymbol{p}_i^2}{2m}+\phi\left(\boldsymbol{r}_i\right)\right]+\sum_{1\le i<j\le N}u_{ij}\left(\boldsymbol{r}_i,\boldsymbol{r}_j\right), \tag{5}$$

where H_N is the Hamiltonian of an N particle system; $\boldsymbol{p}_i^2/2m$ and $\phi\left(\boldsymbol{r}_i\right)$ are the kinetic energy and potential energy, respectively, for the particle in the displacement $\boldsymbol{r}_i$ alone, and $u_{ij}\left(\boldsymbol{r}_i,\boldsymbol{r}_j\right)$ is the interaction energy between the particles.

The two potentials are completely different, and this difference increases when the external field is increased; however, in the absence of an external field, there is no distinction between the two.

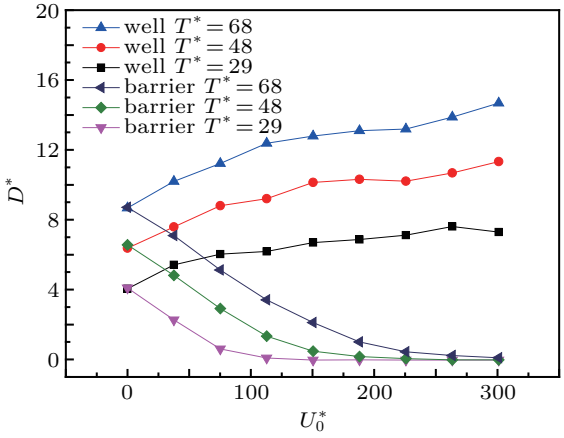


Fig. 2. (color online) Relationship between the external potential field and the diffusion coefficient under the temperatures of 300 K, 500 K, and 700 K. From the diagram, the potential wells and barriers coincide when the potential is 0. The potential well is good for particle motion and diffusion coefficient, while the potential barrier hinders particle transport and decreases the diffusion coefficient.

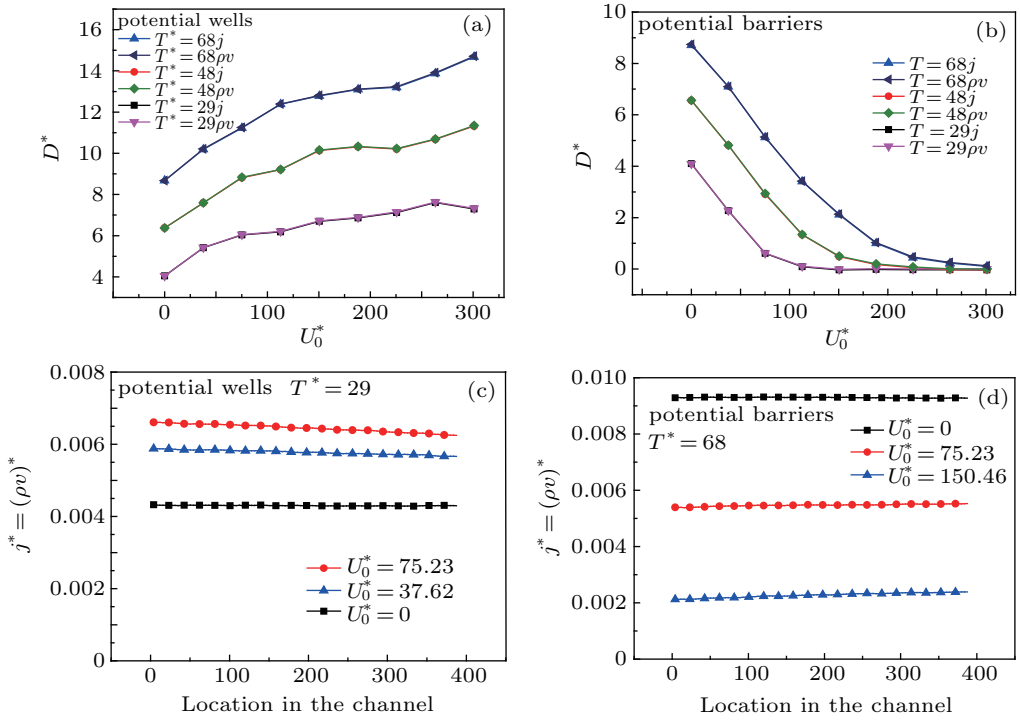


Fig. 3. (color online) (a) We use the density and velocity of each small section of the channel in the potential well. For comparing the actual flux—$\boldsymbol{j}$, the density and velocity are multiplied to obtain the other flux of each section, then the average for the entire channel is obtained. The two values of flux obtained from different ways are in agreement. Then $\boldsymbol{j}$ is translated into D^*. (b) This result also occurs in the potential barrier. Thus, we verify $\boldsymbol{j}=\rho\cdot\bar{\boldsymbol{v}}$ in the transport with external fields. Besides, in the transport channels of the potential well (c) and barrier (d), the products $\rho\bar{v}$ of density and velocity in the entire channel are still almost constants.

Each N particle system in a non-equilibrium state is described by a $2iN$ dimensional phase space, where i is the degree of freedom and N represents the number of parameters for displacement and momentum (velocity, if it is the same kind of particles). In order to understand why the system in a stationary state under different external potentials has different flux tendencies, it is necessary to introduce a core equation: $\boldsymbol{j} = \rho \cdot \bar{v}$, in which $\boldsymbol{j}$ is the flux, ρ is the density, and $\bar{v}$ is the average velocity of the particles. The particle's stream makes the spatial distribution even; the particle's collision makes the velocity even. Due to the non-equilibrium stationary state, $\boldsymbol{j}$, ρ, and $\bar{v}$ are constants in the transport channel according to the coherent principle.

From the figures, it can be seen that $\rho\bar{v}$ is exactly equal to the flux. The diffusion process under an external force is too abstract to perform a theoretical analysis; however, this equation suggests dividing the flux into density and average velocity. An analysis of the particle distribution and velocity statistics could explain how external forces contribute to diffusion.

Introducing the particle distribution visually may be an effective or better way to comprehend the diffusion under the potentials. From the particle distribution shown in Fig. 4, it can be seen that the shape of the graphs almost corresponds to the mathematical function of the potentials.

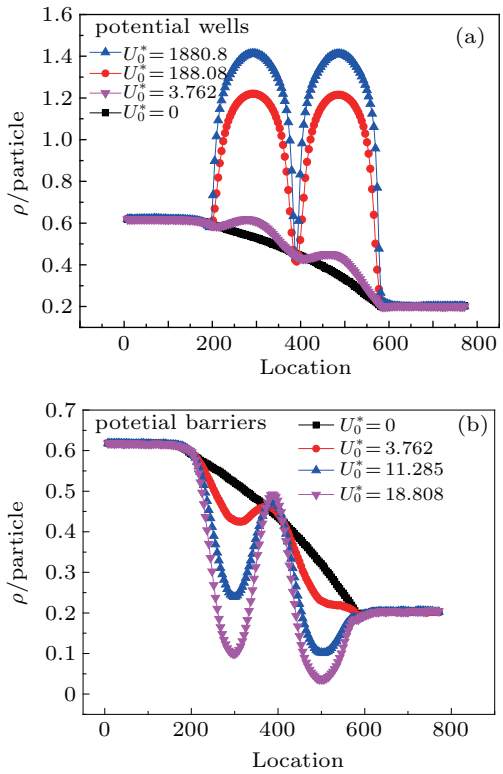


Fig. 4. (color online) Density distribution of the particles in the 200-nm long model. 200 pieces were segmented from the model and the middle 100 pieces were segmented from the channel. The periodic number of the potential field is 2.

The two sides are the particle reservoirs having constant concentrations. If there is no force, the distribution from the high concentration region to the low concentration region will be so smooth without any fluctuation. When the force is not very large, the distribution attains the shape of the external field, but it is still close to the free diffusion. Conversely, when the force is considerable, the shape is dominated by the external field, because of the probability distribution, which was introduced in Ref. [35], and then all the peaks will be near the horizontal line.

From the distribution shown in Fig. 4, it is seen that the external field is supposed to compete with the differential concentration, since the distribution approaches the shape of the potential when the force is increased. On the other hand, the distributions are entirely different when the potential is due to the barrier or the well. When the force is enhanced, the potential barrier arches more pointedly and the well sinks more deeply, so the barrier stores less particles and the well stores more particles. We use this assumption as the reason why the collective diffusion is related to the external potential field.

If the particles are propelled only by the concentration gradient without any external force, it is the classical non-equilibrium condition. However, the concentration gradient can be ignored as the detailed balance when the external field is large enough to the concentration gradient. If the canonical ensemble distribution function is assumed to be dominant, then problem can be managed by the equilibrium theory in the microscopic local scheme. In such a non-equilibrium stationary state and its constant distribution, the number of particles that flow into a local position equals the same as that flowing out; the number of particles fluctuates around a theoretical value. The probability distribution function, which describes the population of identical particles in the equilibrium state, is given by

$$P \sim \exp\left(-\frac{-\Delta W(x)}{kT}\right), \tag{6}$$

where k is the Boltzmann's constant, T is the medium temperature, x is an arbitrary set of coordinates, and $W(x)$ is the minimum reversible work required to change the state,[35] which is related to the maximum useful work that can be extracted from it. $W(x)$ includes the L–J potential to repel each particle. Its calculation is very complicated, therefore, the theoretical results rely on the simulation.

For simplification in the local scope, the particle velocity distribution can be considered to approach the Maxwell velocity distribution in equilibrium[36]

$$f^{(0)}(\boldsymbol{r},\bar{\boldsymbol{v}},t) = n_{\mathrm{loc}}\left(\frac{m}{2\pi kT}\right)^{i/2} \times \exp\left[\frac{-m}{2kT}(\boldsymbol{v}-\langle \boldsymbol{v}(\boldsymbol{v}(\boldsymbol{r},t)\rangle)^2\right], \tag{7}$$

where i is the degree of freedom, m is the particle mass, T is the temperature, k is the Boltzmann's constant, $\boldsymbol{r}$ is the

location, $n_{\rm loc}$ is the local density, $\boldsymbol{v}$ is the velocity, t is the time (however, stationary state is independent of time), and $\langle \boldsymbol{v} \rangle$ is the local average velocity. Assuming local equilibrium, $n_{\rm loc}(r,t)$ and $\langle \boldsymbol{v}(\boldsymbol{r},t) \rangle$ are functions of location and time.

In our results, the average transport velocity was only several meters per second, and the local average velocity was just less than thirty meters per second. Both were less than the usual particle velocity, which is why we omitted the local average velocity and compared the results with the Maxwell velocity distribution directly.

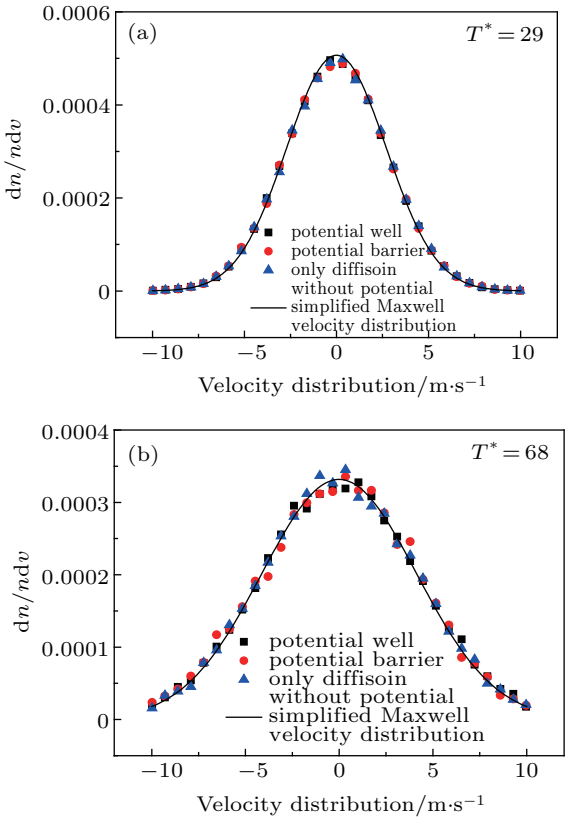


Fig. 5. (color online) In the velocity distribution of potential well, potential barrier, and only diffusion without potential, these (a) 300 K and (b) 700 K temperature conditions are similar to those of the Maxwell velocity distribution. The fitting curves of the rate points have a little deviation to the zeroth symmetrical axis and this deviation is about the drift velocity.

The Maxwell velocity distribution, which can also be applied for non-ideal gas, conforms exactly with the transport under low drift velocity condition. The probability of particle velocity accords with the Maxwell velocity distribution, irrespective of the external potential, internal force, and average drift velocity.

The average transport velocity is usually decided by the temperature and concentration difference. The average velocity statistics and total particle number of the entire channel is calculated, as shown in Fig. 6.

According to statistical mechanics, when the external potential is introduced, the higher energy level gets fewer particles and the lower energy level gets more particles, even though the mutual L–J potential impedes to some extent. As the potential well has a lower energy level than the two reservoirs, more particles occupy the wells, which means that the potential well is the surrounding for mass transfer. In the opposing surrounding, the potential barriers are occupied by fewer particles, because of its higher energy level, which implies that it is a hindrance for transport. As $\boldsymbol{j} = \rho \cdot \bar{v}$, higher density results in a greater flux. On the other hand, for potential barriers, increasing the external potential reduces both the variables — total density and average velocity.

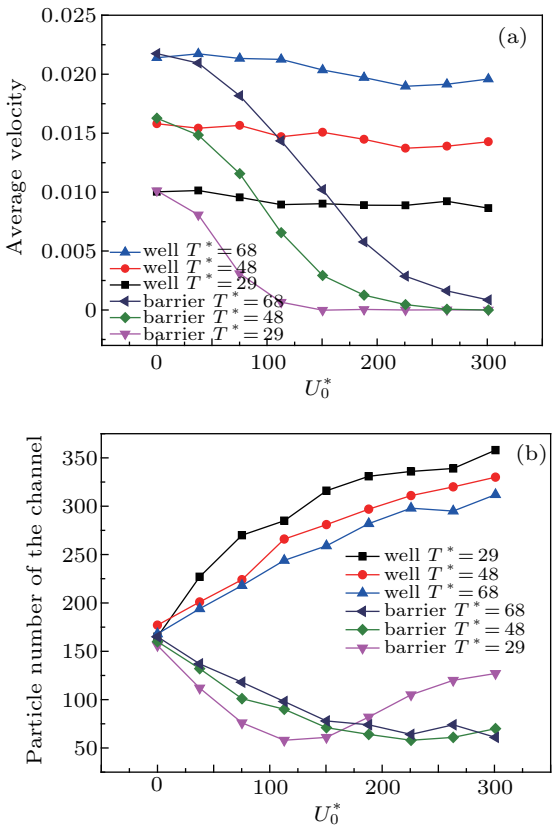


Fig. 6. (color online) (a) Average velocity; the higher the temperature, the higher the average velocity. Besides, the potential strength has little effect on the velocity in the potential well. (b) Particle number; the changes in temperature and potential type are in accordance with the tendency in the Boltzmann distribution. Density is the main factor for diffusion.

Some other works have studied the other factors. Even though some tendencies are similar, there are different performances depending on the external force.

Figure 7 illustrates the relationship between temperature and diffusion coefficient under different potentials. The temperature ranges from 150 K to 500 K. The diffusion coefficient increases in direct proportion to the temperature, regardless of wells or barriers. For potential wells, the diffusion coefficient increases with an increase in the amplitude of force; for potential barriers, the diffusion coefficient decreases with an increase in the amplitude of force. When the amplitude becomes 0, the two lines converge.

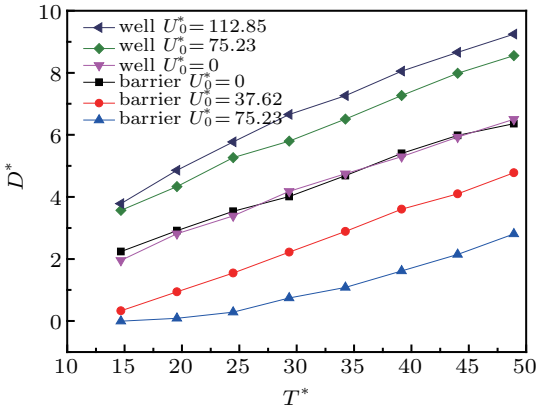


Fig. 7. (color online) Temperature dependence of the collective diffusion coefficient for different potentials.

It is not difficult to understand why a warming temperature is favourable for diffusion from the perspective of particle activity and rate. Einstein gave a relationship between dissipation and position fluctuation in 1905: $\zeta D = kT$, where ζ is the frictional coefficient, which is constant in this system. It clearly indicates that D varies linearly with temperature.

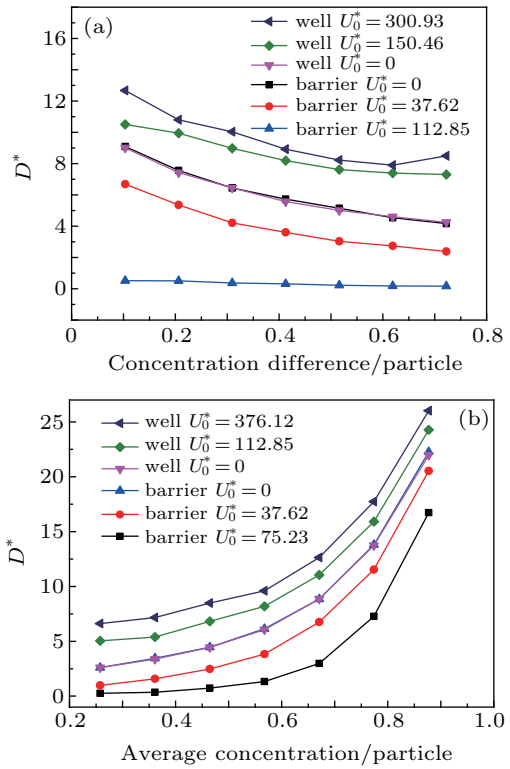


Fig. 8. (color online) (a) Concentration difference; one reservoir is regulated as 160 particles and in the other reservoir it is changed from 20 to 160. Even though all lines have downward slopes, the data of flux also show that particle flux is increased with increase in concentration, difference; (b) the difference in number of particles between the two reservoirs is maintained as 20. The number of time steps of the programs is set as 5×10^9 for (b)

Figure 8 illustrates the dependence of diffusion on concentration difference and average concentration, for different values of potential. From Fig. 8(a), which shows the effect of concentration difference, it can be seen that the diffusion coefficient decreases with the increase in concentration difference. In Fig. 8(b), it can be seen that the diffusion coefficient increases with an increase in the average concentration. Figure 8 indicates that barriers and wells have the same tendency, but the diffusion ability of the potential well is better than that of the potential barrier.

More particles come with larger flux. It indicates that the diffusion coefficient increases with average concentration. In the case of concentration difference, Fick's law states that the difference in concentration is the favourable condition for transport, as indicated by the rate of flux.

In Fig. 9(a), it is seen that there is a small curl in the area of the relatively shorter channel, which indicates ballistic transport; however, it has a steady value in the long channel, which indicates diffusive transport.[32,37] In most parts of Fig. 9, the diffusion coefficient is steady.

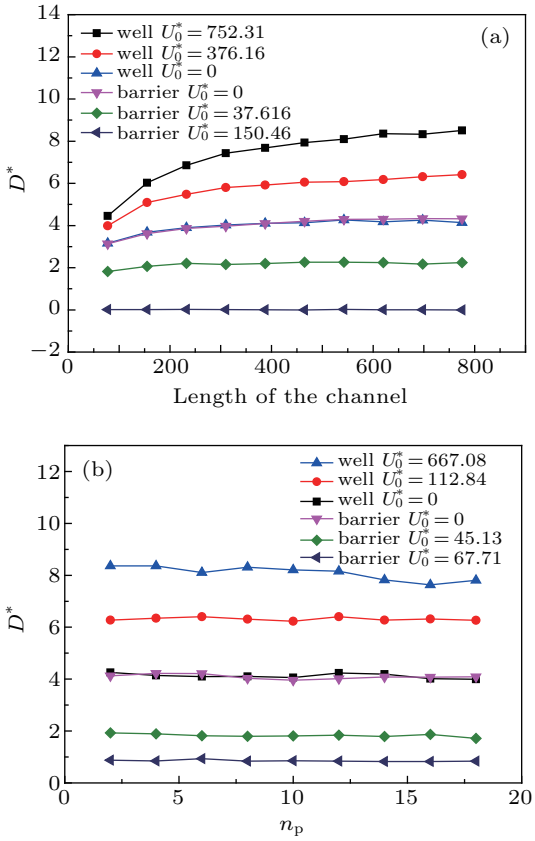


Fig. 9. (color online) These two figures imply that neither the (a) length of transport channels nor the (b) period of force fields can affect the transport. For this part, the potential field need to be amended, because of the invariance of the potential depth or height through changing variables.

Linear fitting was performed in Fig. 9, and it exhibits that the channel length and the force period contribute to the collective diffusion.

5. Conclusion

Finally, the following conclusions can be drawn about the collective transport under external potential. In all the above

diagrams, there is one common factor — the situation of wells and barriers coincide when the external force becomes zero, which validates our results. This phenomenon can be explained by the canonical ensemble distribution, Boltzmann relationship, Einstein relation, etc.

Potentials affect the transport, even though additional potentials do not change the potential energy of the two reservoirs. Two contrary potentials — the potential well and the potential barrier — represent two contrary conditions of transport. All the above diagrams indicate that the potential well is an active driver for the collective diffusion of particles, while the potential barrier is an obstacle.

The system is combined with different fields, where the external force field, concentration field, and internal particle potential couple and tangle together. In addition, statistical analysis and subsection method were used to divide the flux into density and velocity. External potential affects the distribution function of Gibbs relation; however, the L–J potential impedes to some extent. In general, a higher particle density indicates greater particle transport.

In particular, the Maxwell velocity distribution, as the generally acknowledged principle, is still applicable to the approximate equilibrium state.

Other surroundings such as the temperature, concentration difference, and average concentration, are the subordinating parameters; therefore, the coefficients have the same tendency, irrespective of the type of potential. The length of the transport channel and the period of the external field have a delicate influence on diffusion.

The creation of this research is to divide the flux into density and velocity, which relate to the sectional statistics of position and momentum. The results show that these two kinds of distributions approach the equilibrium state. This analytical method of dividing the flux, which could be referenced in similar problems, successfully answers the questions of why and how the potentials influence the mass flux. From an academic perspective this study enriches the non-equilibrium theory, verifies the relevant knowledge, and provides theoretical explanations. In the subcellular level, particles always confront the external force. This transport model is also based on simulation, and we hope that this work can provide some numerical references in homologous areas such as controlling the flux by controlling the external potential. Particularly, in biology, for instance, the selectivity filter or protein channel are similar to physical systems. Creatures live in the non-equilibrium state. Fick's law, which is a popular transport law, still faces difficulty in solving any real non-equilibrium problem, especially in biology. With the help of the diffusion simulation, this study may be a guide or reference for the analysis of molecular transports.

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