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SPECIFIC FEATURES OF THE SIMULATION OF THE PARTICLE DIFFUSION PROCESSES IN SPATIALLY PERIODIC FIELDS[†]

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This paper is devoted to the studies of the specific features of the simulation of the particle diffusion processes in space – periodic potentials using Langevin equations. Different methods used for the presetting of initial conditions and their effect on the obtained solutions have been analyzed. It is shown that the system is nonequilibrium for all the methods of the presetting of initial conditions during a certain time interval of t_{trm}. This interval is increased as $1/\gamma$ with a decrease in the friction coefficient. A reasonable description of the transient processes of particle transport and diffusion requires a preliminary system thermalization procedure. A new method of the presetting of initial conditions that provides the most accurate description of equilibrium system has been suggested. It consists in the generation of the initial particle coordinates and velocities that correspond to the equilibrium distribution of harmonic oscillators with a specified temperature. The use of such initial conditions enables the computations with a good accuracy using no thermalization procedure at $T < 0.1$. The classic method of the determination of diffusion coefficients D as a limit $\lim\limits_{t\to\infty}\left(\sigma^2/2t\right)$ has been analyzed. It was shown that the use of it for computer-aided calculations is limited by the restricted computational time. It results in that the computation of D under certain conditions becomes impossible. A new method was suggested for the determination of the diffusion coefficient using the linear approximation of the dependence of dispersion on time. This approximation can only be possible after the kinetic temperature attains its stationary value. The suggested method requires several orders of magnitude less time in comparison to the classic method. As a result, it enables the computation of the diffusion coefficient even in the cases of total previous failure. The obtained data are of great importance for correct simulation computations of diffusion processes and for the appropriate physical interpretations of obtained data.

Keywords: diffusion, computer simulation, Langevin equations, initial conditions, external fields.
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Particle transport and diffusion processes in periodic potentials that are exposed to the action of external fields play an important role for different phenomena peculiar for physics, chemistry and biology [1-2]. For example, Josephson junctions [3], superionic conductors [4], Josephson Vortex [5], charge density waves [6], magnetic ratchets [7], granular gas [8], surface diffusion [9], optic vortexes [10] and the membrane permeability [11], actually it is by far incomplete list of mentioned phenomena.

Recently, a substantial progress was achieved in the analytical studies of the particle transport and diffusion in the overdamped state [12-13]. At the same time, the developed methods are poorly acceptable for low dissipation systems. In this connection, the methods of computer simulation were intensively used along with analytical computations. In particular, the numerical solution of Langevin equations [14-18] has intensively been used.

Numerical solution of stochastic equations has the specific features of its own that are relating both to the presetting of initial conditions and the limited simulation time. The temporal dynamics of the obtained values of the diffusion coefficient and the particle mobility in the transient state depend to a great extent on the type of initial conditions. And the time limitation has an effect on the correct definition of such values as the mobility and the diffusion coefficient.

The purpose of this scientific paper was to evaluate already available methods and develop new efficient methods for the presetting of initial conditions and analyzing the solutions of stochastic Langevin equations.

BASIC RATIOS AND SIMULATION METHODS

The Langevin equation is usually used for the simulation of the motion of Brownian particles in the periodic potential exposed to the action of external fields:

$$m\ddot{X} = -\frac{d}{dx}U(X) - g\dot{X} + F(\tau) + \xi(\tau), \tag{1}$$

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where X is the particle coordinate, m is the particle mass, τ is the time, g is the friction coefficient, and $F(\tau)$ is the external force. The dot on top denotes the time differentiation. The term $\xi(t)$ describes thermal fluctuations. The noise is a white Gaussian noise and accordingly the ratio of

$$\langle \xi(t)\xi(t')\rangle = 2gk\Theta\delta(\tau-\tau'), \tag{2}$$

where k is the Boltzmann constant and Θ is the temperature.
For the potential particle energy in the periodic potential with period L the relation of

$$U(X+L)=U(X). \tag{3}$$

is true. Henceforth, we will make use of the most frequently used type of the periodic potential, in particular

$$U(X)=-\frac{U_0}{2}\cos\left(\frac{2\pi}{L}X\right) \tag{4}$$

where U_0 is the potential barrier height.

The moving particle is exposed to the action of the periodic force exerted by the lattice F_{lat} :

$$F_{lat}=-\frac{dU}{dx}=F_0\sin\left(\frac{2\pi}{L}X\right). \tag{5}$$

The period of low natural vibrations in such a potential is equal to $\tau_0=L(2m/U_0)^{1/2}$.

It is convenient to change over to dimensionless values to analyze the simulation data [1,19]. Let's apply the transformations:

$$x=\frac{2\pi}{L}X \quad , \quad t=\frac{\tau}{\tau_0} \ . \tag{6}$$

By selecting mass units $m=1$, $k=1$, we obtain a maximum simple type of the equation (1):

$$\begin{gathered}\ddot{x}=-\sin x-\gamma\dot{x}+f(t)+\zeta(t),\\ \langle\zeta(t)\zeta(t')\rangle=2\gamma T\delta(t-t'),\end{gathered} \tag{7}$$

Dimensionless units are relating to the force through the friction coefficient and temperature as follows:

$$\gamma=G\frac{\tau_0}{2\pi m} \quad , \quad f(t)=\frac{F(t)}{F_0} \quad , \ T=\frac{2k\Theta}{U_0} \tag{8}$$

To evaluate the extent of the thermal equilibrium of the system described by equations (7) we will use the kinetic temperature that is often used by the nonequilibrium statistical physics [20]:

$$T_{kin}=\frac{m}{k}\langle\Delta v^2\rangle \tag{9}$$

Here, the brackets denote the ensemble averaging and $\langle\Delta v^2\rangle=\langle(v-\langle v\rangle)^2\rangle$ denotes the velocity variances. In the state of thermal equilibrium the kinetic temperature of the system is equal to the thermostat temperature of $T_{kin}=T$.

The particle transport will be characterized by the value of the average velocity of the particle ensemble:

$$\langle v\rangle=\int_{-\infty}^{\infty}vn(v)dv \tag{10}$$

where $n(v)$ is the normalized function of the particle velocity distribution.

To analyze diffusion processes we will use the dispersion for the particle coordinate distribution:

$$\sigma^2(t) = \left\langle \left(x(t) - \langle x(t) \rangle \right)^2 \right\rangle \tag{11}$$

Stochastic equation (7) was solved numerically for each particle using stochastic Heun algorithm [21]. The time step was equal to 0.01. The statistical ensemble averaging was carried out for the particle number of at least $N = 5 \cdot 10^4$.

ANALYZING INITIAL CONDITIONS

In order to solve equation (7) we need to preset appropriate initial conditions. These conditions should conform to the described physical situation. When exposing the particles to the action of different external fields we usually assume that these are in thermal equilibrium with the thermostat. It allows us to get rid of wrong physical inferences due to the superposition of two different processes, in particular thermalization and the external field action.

Let's consider different boundary conditions for the simplest case of $f(t) = 0$ when the external force is unavailable. The condition of

$$x(0) = 0; v(0) = 0, \tag{12}$$

is realized in the easiest way and it was used, for example, in paper [22]. In this case, curve 1 in Fig. 1 shows a change in T_{kin} in time. The diagram shows that the kinetic temperature at initial times is considerably lower than T. The system comes to the thermal equilibrium during the thermalization period. It can be seen in Fig. 2 that the drop in temperature has no strong effect on this phenomenon. Hence, after the time $t > t_{trm}$ thermalization processes will have no effect on the behavior of the particle ensemble exposed to the external force action. However, at $t < t_{trm}$ the system is artificially cooled and it fails to comply with the condition of thermal equilibrium.

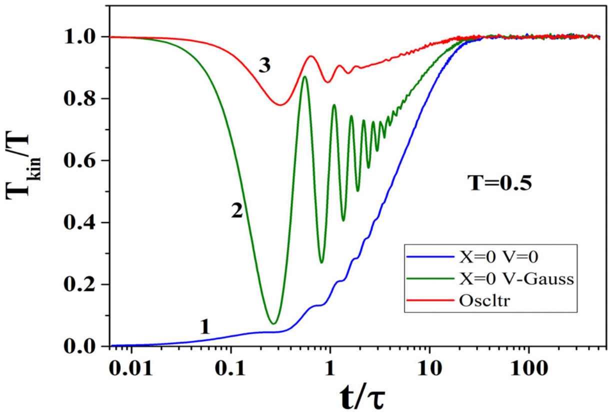

Figure 1. The dependences of the kinetic temperature T_{kin} as a function of time for different initial conditions. T = 0.5 1 – initial conditions (12), 2 – initial conditions (14), 3 - initial conditions (24). $\gamma = 3 \cdot 10^{-2}$.

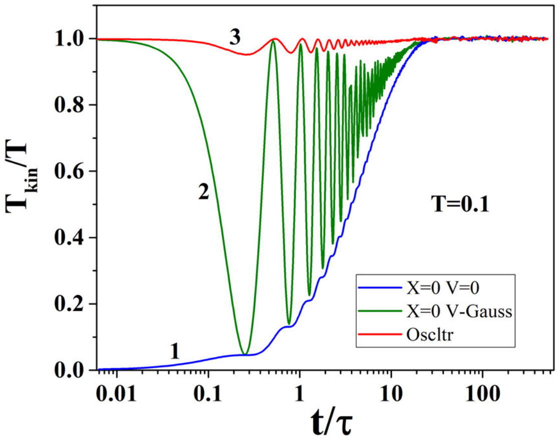

Figure 2. The dependences of the kinetic temperature T_{kin} as a function of time for different initial conditions. T = 0.1 1 – initial conditions (12), 2 – initial conditions (14), 3 - initial conditions (24). $\gamma = 3 \cdot 10^{-2}$.

The conditions that are frequently used are the presetting of initial velocities and the coordinates that are distributed in some physical space domain [23-24] independently of the thermostat temperature. Fig. 3 shows a change of T_{kin} in time for the case when the initial coordinates and velocities are uniformly distributed as:

$$x(0) = Unif(0, 2\pi), \\ v(0) = Unif(-1.0, 1.0), \tag{13}$$

where $Unif(a, b)$ is the uniformly distributed random value in the interval from a to b.

The curves 1 and 2 correspond to the thermostat temperatures of $T = 0.1$ and $T = 0.5$, accordingly. The Figure shows that in both cases T_{kin} exceeds the thermostat temperature by several times at $t < t_{trm} \approx 30\tau$. The lower the thermostat temperature the more T_{kin} exceeds T. Hence, before the time $t < t_{trm}$ we deal with the substantially overheated system.

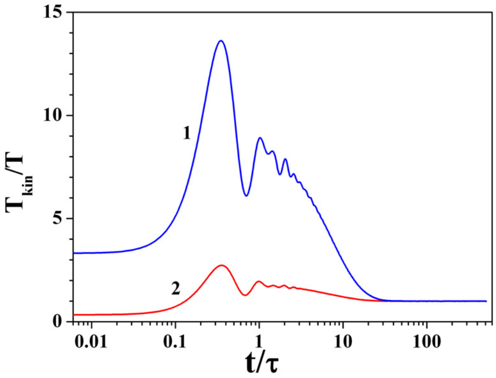

Figure 3. The dependences of the kinetic temperature T_{kin} as a function of time for initial conditions (13). $\gamma = 0.03$.
1 – T = 0.5, 2 – T = 0.1.

Most frequently, initial conditions are preset in the following manner: all the particles are organized at the origin of coordinates $x(0)=0$, and then these are imparted initial velocities that correspond to the equilibrium Maxwell velocity distribution [25]:

$$\begin{aligned} &x(0)=0, \\ &p(v)=\chi\exp\left(-mv^2/(2kT)\right), \end{aligned} \tag{14}$$

where χ is the normalization coefficient. In this case, in spite of the fact that the particle velocity distribution function really corresponds to the equilibrium function, the equilibrium particle coordinate distribution has not been realized. Curve 2 in Fig 1 demonstrates this fact. The value of T_{kin} is below the thermostat temperature and it oscillates with a higher amplitude before the time of t_{trm} is achieved. Fig. 2 shows that a drop in T_{kin} results in an increased oscillation amplitude of T_{kin}/T . Hence, using the initial conditions specified in (14) we also deal with the “frozen” system that is far from the equilibrium state.

It can be seen from the above that all available methods result in the strong deviation of the system from the equilibrium within t_{trm} . Hence, the use of the boundary conditions (12)-(14) requires the conduction of the thermalization procedure during the studies of transient processes when the system is exposed to the action of external fields, as it was done, for example, in scientific paper [26].

To put things right, we suggest new initial conditions that are the closest to the equilibrium for the particles in the spatially periodic potential. Under these conditions, we suggest to view the initial particle ensemble as the system of harmonic oscillators that is in the thermal equilibrium with the thermostat. Assuming that these are small-amplitude oscillations observed near the potential well bottom the harmonic oscillator motion equation can be written as:

$$\ddot{x}+\omega_0^2 x = 0 \, , \tag{15}$$

where ω_0 = is the natural frequency of small-amplitude oscillations:

$$\omega_0^2 = \alpha \, , \tag{16}$$

and $\alpha = \dfrac{1}{2}\dfrac{d^2U(x)}{dx^2}$ corresponds to the potential “stiffness”.

It is a well-known fact that the equation (14) has the solution

$$\begin{aligned} &x(t)=A\sin(\omega_0 t+\varphi), \\ &v(t)=\dot{x}=A\omega_0\cos(\omega_0 t+\varphi), \end{aligned} \tag{17}$$

where A is the oscillation amplitude of the oscillator. The oscillator energy is equal to

$$E=\alpha A^2/2. \tag{18}$$

In the state of heat equilibrium the particle energy distribution has the Boltzmann distribution form:

$$p(\varepsilon) = \beta \exp\left(-\frac{\varepsilon}{kT}\right), \tag{19}$$

where β is the normalization factor derived from the statement that

$$\int_0^\infty p(\varepsilon) d\varepsilon = 1, \tag{20}$$

To obtain initial particle coordinate and velocity distributions the following algorithm should be realized:

1) Using the distribution (19) we find a random energy ε for each particle that obeys the exponential distribution with the mathematical expectation equal to kT:

$$\varepsilon = -kTLn(r_1), \tag{21}$$

where r_1 is a random number uniformly distributed in the interval of [0,1].

2) Using (18), we compute the oscillation amplitude value A:

$$A = \sqrt{\frac{2\varepsilon}{\alpha}}, \tag{22}$$

3) phase φ is considered equivalent to the random number r_2 that is uniformly distributed in the interval ranging from 0 to 2π:

$$\varphi = r_2, \tag{23}$$

4) Using the expression (17) at the initial moment of $t = 0$ we compute initial particle coordinate and velocity values:

$$\begin{aligned} x(0) &= A\sin(\varphi), \\ v(0) &= A\omega_0 \cos(\varphi). \end{aligned} \tag{24}$$

In Fig. 1-2, the curves 3 correspond to initial conditions (24). The diagrams show that initial conditions (24) are the closest to thermal system equilibrium conditions. In other words, it is preferable to use initial conditions (24) for the analysis of the systems in which the particles were in the heat equilibrium state. Fig. 4 shows the deviation from the heat equilibrium under these initial conditions for different temperatures. The Figure shows that in contrast to other initial conditions a drop in temperature results in the lessening of the deviation from the equilibrium distribution. At $T \le 0.1$, the kinetic temperature T_{kin} differs from the thermostat temperature within 4%.

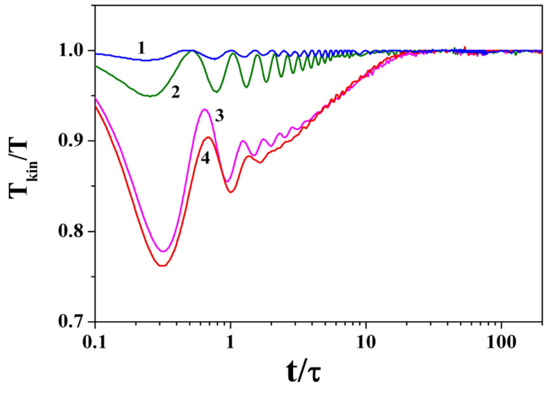

Figure 4. The dependences of the kinetic temperature T_{kin} as a function of time for different T values. Initial conditions (24). $\gamma = 0.03$. 1– T = 0.01, 2 – T = 0.1, 3 – T = 0.5, 4 – T = 1.0.

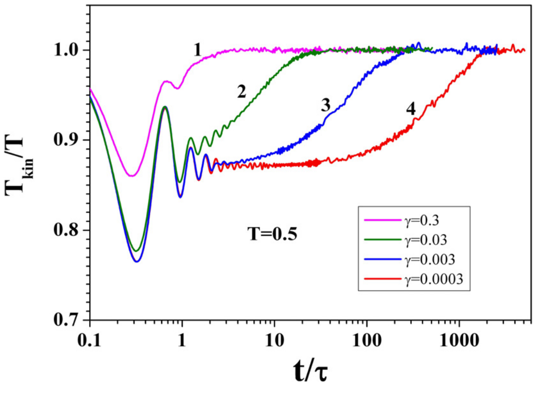

Figure 5. The dependences of the kinetic temperature T_{kin} as a function of time for different γ values. Initial conditions (24). T = 0.5. 1– γ = 0.3, 2 – γ = 0.03, 3 – γ = 0.003, 4 – γ = 0.0003.

Let's consider a change in t_{trm} depending on the dissipative properties of the system. Based on the above, since initial conditions (24) are the closest to equilibrium conditions we will confine ourselves to their studies. Fig. 5 gives a change in the value of T/T_{kin} for different values of γ. The Figure shows that the thermalization time is linearly increased with a decrease in γ. While for $\gamma = 0.3$ it is equal to $t_{trm} \approx 3$, for $\gamma = 0.0003$ it is increased to $t_{trm} \approx 3000$. Hence, the value of t_{trm} is increased as $1/\gamma$ with a decrease in the friction coefficient. The use of initial conditions (24) enables high accuracy computations using no thermalization procedure at temperatures of $T < 0.1$. Under other conditions it is recommended to carry out the thermalization procedure.

CALCULATING THE DIFFUSION COEFFICIENT

The correct computation of the diffusion coefficient D is a vital problem for many investigations. A classic method of the determination of D for computer-aided calculations consists in the direct use of the definition of the diffusion coefficient as [27-28]:

$$D = \lim_{t\to\infty} D_{ef}(t) = \lim_{t\to\infty} \frac{\sigma^2}{2t} = \lim_{t\to\infty} \frac{\left\langle \left(x - \langle x \rangle\right)^2 \right\rangle}{2t}. \tag{25}$$

A key question put in the papers highlighting computer simulations is what estimated time we should confine to? Usually, the time is selected so that the clear-cut linear dependence of $\sigma^2(t) = 2Dt$ is observed in the log-log scale, for example as for t > 10^6 in Fig. 6. This Figure gives the example of a change in the dispersion value with time under the action of the constant force [29]. Fig. 7 gives curve 2 that corresponds to the dependence of $\sigma^2(t)/t$.

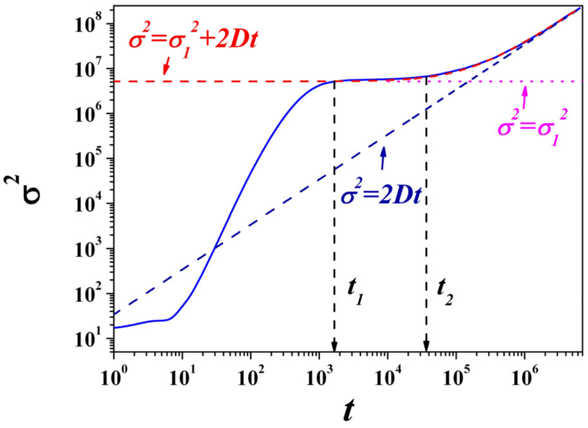

Figure 6. The dependence of the dispersion on time under the action of constant force $f = 0.25$. $\gamma = 0.3$, T = 0.5. The solid line is the simulation data. The dash-dotted line is $\sigma^2 = 2Dt$ asymptote, the dashed line shows the approximation $\sigma^2 = 2Dt + \sigma_1^2$, and the dotted line shows constant σ_1^2. The arrows show the starting and the ending time of the “dispersionless” phase.

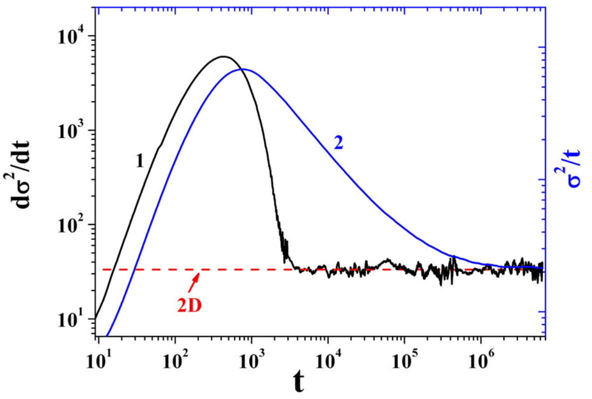

Figure 7. The dependence of $d\sigma^2/dt$ (curve 1) and σ^2/t (curve 2) on time. The dashed line shows the value of $2D$. $f = 0.25$, $\gamma = 0.3$, T = 0.5.

Apparently, to obtain the right value of D using the formula (25) we need time t > 10^6. As is seen from Fig. 6 the dependence of $\sigma^2(t)$ shows the presence of the horizontal “plateau” between the times t_1 and t_2. It is the so-called phase of the “dispersionless” transport [30]. With a drop in temperature the duration of it is exponentially increased [29]. It makes impossible to derive D from formula (25) during a reasonable computational time in many cases. Specifically, in paper [31] the authors failed to define the value of D in the force interval of F = 0.2-0.9. However, as is shown in [29] in spite of the formation of the exponential particle coordinate distribution in the phase of the “dispersionless” transport this phase is characterized by the ordinary diffusion with $\sigma^2(t) \propto t$. To make it more apparent, let’s appeal to Fig. 7.

The Figure shows the time dependence of $d\sigma^2/dt$. It appears that if we use the differential definition of the time-dependent diffusion coefficient $D(t)$ [32-33]

$$D(t) = \frac{1}{2}\frac{d\sigma^2}{dt}, \tag{26}$$

the mean value of $D(t)$ don’t change at $t > t_1$. Only thermal fluctuations are observed near the mean value. It means that at $t > t_1$ we deal with the ordinary diffusion. For the sake of clarity let’s venture into Fig. 8.

It gives the diagrams of the time dependence $\sigma^2(t)$, $T_{kin}(t)$ and $\langle v \rangle(t)$. It can be seen that the superdiffusion phase is ended at $t \approx t_1$ and the ordinary diffusion phase with $\sigma^2(t) = \sigma_1^2 + 2Dt$ is originated. As was shown in [29], the value of σ_1^2 is defined by the duration of the superdiffusion phase. The end of the superdiffusion phase is characterized by the establishment of the stationary value $T_{kin}(t)$. In addition, a stationary distribution of $\langle v \rangle(t)$ is established at $t > t_1$. As is seen in Fig. 7 the dependence of $d\sigma^2 / dt = const$ is established at the same time. Hence, the establishment of the stationary value $T_{kin}(t)$ is indicative of the beginning of the phase of ordinary diffusion with $\sigma^2(t) \propto t$.

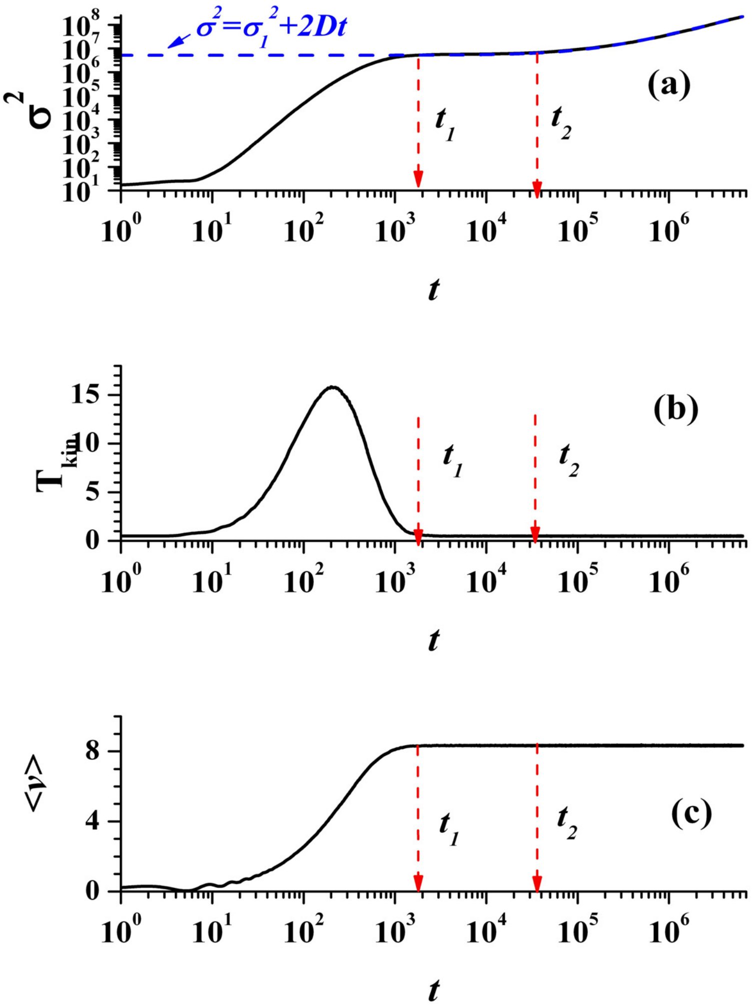

Figure 8. The dependence on time versus a) dispersion; b) the kinetic temperature; c) average velocity under the action of the constant force $f = 0.25$. $\gamma = 0.3$, T = 0.5. The dashed line shows the approximation $\sigma^2 = 2Dt + \sigma_1^2$.

As is shown above, the diffusion factor can be calculated using the time-averaged value (26) at $t > t_1$.This method has its drawbacks relating both to numerical differentiation procedure complications and the use of this method for other situations in addition to $f(t) = const$.The integral method is more stable and it enables an easy computation of the diffusion factor already during the time of the “dispersion-free” transport. It follows from the consideration given above that after the attainment of time t_1

$$\sigma^2(t) = 2Dt + \sigma_1^2 \text{, at } (t > t_1), \tag{27}$$

It was shown in [29] that σ_1^2 is exponentially increasing with the drop in temperature. Therefore, the second term in (27) will dominate over the first term for a rather long time. However, in the case of the fitting of $\sigma^2(t)$ data by the dependence (27) with free σ_1^2 and D parameters using the least square method we can obtain the diffusion factor with a high accuracy already at short times.

Let’s get back to Fig. 6. Using the relation (25) for time t = $6.4 \cdot 10^6$ we obtain D = 17.30. With an increase in time by one order of magnitude we get D = 17.06 at t = $6.4 \cdot 10^7$. In other words, it takes a rather long time to get the diffusion coefficient with a high accuracy. Taking into consideration the exponential growth of $\Delta t = t_2 - t_1$ with a drop in temperature [29] we can draw a conclusion that it is impossible to derive D for lower temperatures during a reasonable computational time. However, using (27) we can approximate $\sigma^2(t)$ at a considerably shorter time interval, in particular t =1.0·10^4 -5·10^4. Providing the $\sigma^2(t)$ data fitting using the least square method we will see that in this case the dispersion is described by the linear dependence (27) with the correlation coefficient equal to 0.999.

Using the data in this limited time interval we will get the value of D = 17.03. In other words, the use of (27) results in the reduction of the computational time by the factor of 6000 to get the same value of D as proceeding from the expression (25) for time t = 6.4·10^7. With the drop in temperature the required estimated time lag between (25) and (27) will be growing exponentially. And the derivation of the value D proceeding from the expression (25) becomes unrealistic. However, using the data fitting (27) the diffusion factors can easily be derived even in the cases of total previous failure. This approach can also be applied to other systems that show a considerable dispersion growth in the initial phase. However, we must be careful and confident that all the transient processes have already been completed. As an example, let's give some data for the periodic force of the type

$$f(t) = a\sin(\omega t). \tag{28}$$

Fig. 9 gives the data for one of such computations. Fig. 9b shows that at $t > 400$ the system passes into the stationary state and the yield of the stationary value by the kinetic temperature is indicative of it.

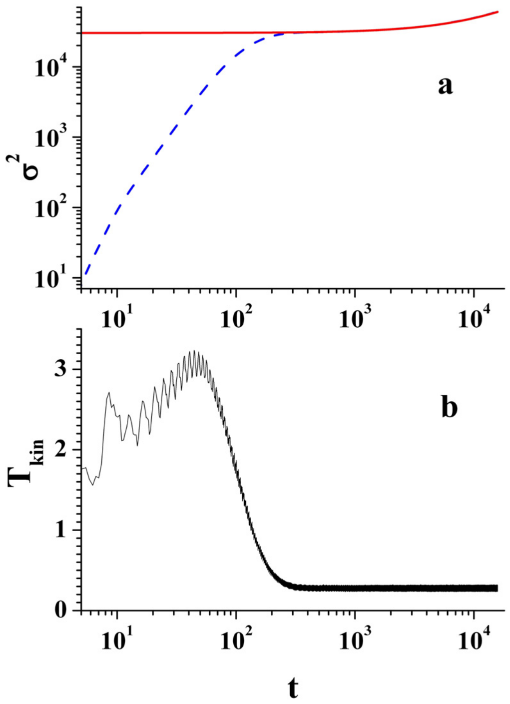

Figure 9. The dependence on time versus a) dispersion; b) the kinetic temperature under the action of periodic external force. The dashed line shows a) the simulation data, the solid line shows the linear approximation. $a = 10.0$, $\gamma = 0.318$, T = 0.2, $\omega = 1.59$.

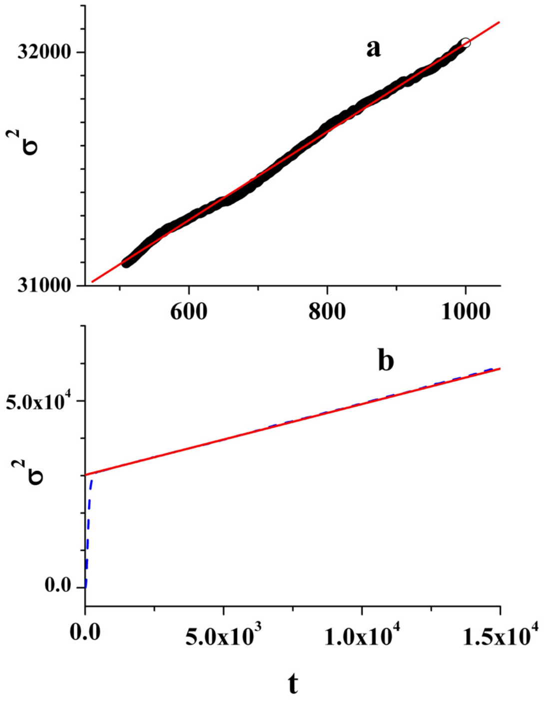

Figure 10. The dependence of σ^2 on time. a) the markers show the simulation data for the ensemble consisting of 50000 particles, the solid line is the linear approximation and the dashed line is the simulation data; b) the solid line is the linear approximation and the dashed line is the simulation data. $a = 10.0$, $\gamma = 0.318$, T = 0.2, $\omega = 1.59$.

Though, the dependence of $\sigma^2(t)$ in Fig. 9a looks like subdiffusion or "dispersionless" transport in these time intervals, however in reality the ordinary diffusion takes place at $t > 400$ as is well seen in Fig. 10b.

In Fig. 10a, the simulation data of the ensemble consisting of 50000 particles are shown by the markers. The solid line shows the linear approximation of these data. The least square method was used for the approximation [34]. Fig. 9a and Fig. 10b show that the linear approximation approximates well the dependence of $\sigma^2(t)$ at $t > 500$ in the limited linear section of Fig. 10a. Fitting the data in Fig.10a by using the linear regression method, we obtain the linear relationship with a correlation coefficient of 0.998. Using the data in the interval of $500 < t < 5000$ we increase the correlation coefficient value to 0.9998. It allows us to derive the diffusion coefficient with a high degree of confidence as 1/2 of the slope at a significantly reduced computational time in comparison to that spent using the classic method.

The abovementioned method used for the derivation of the diffusion coefficient was successfully used by us earlier [35-36]. Therefore, it can be recommended for a wide application by other systems.

CONCLUSIONS

This paper delves into the studies of the specific features of the simulation of the diffusion processes of particles in spatially periodic potentials using Langevin equations. Different methods used for the presetting of initial conditions and their effects on obtained solutions have been analyzed. It was shown that the system is nonequilibrium for all the methods used for the presetting of initial conditions during a certain time interval of t_{trm} .This interval in increased as $1/\gamma$ with a decrease in the friction coefficient. The kinetic temperature with regard to the methods used today for the presetting of initial conditions differs from the thermostat temperature by tens of percent. Hence, the adequate description of the transient particle transport and diffusion processes exposed to the action of external fields requires a preliminary system thermalization procedure during the time of at least t_{trm} .

A new method of the presetting of initial conditions under which the system is close to the thermal equilibrium has been suggested. It consists in the generation of the initial particle coordinates and velocities that correspond to the equilibrium distribution of harmonic oscillators at a specified temperature. The use of these initial conditions enables the computations using no thermalization procedure at the temperature of $T < 0.1$ with the error less than 4%.

A classic method of the computation of diffusion coefficients D as a limit $\lim_{t\to\infty}\left(\sigma^2/2t\right)$ has been analyzed. It was shown that the use of it for computer-aided calculations is limited by the restricted computational time. It makes the computation of D impossible under certain conditions. A new method was suggested for the determination of the diffusion coefficient through the linear approximation of the dispersion versus time dependence. This approximation is only possible after the kinetic temperature attains its stationary value. The proposed method requires several orders of magnitude less time in comparison to the classic method. As a result, it enables the computation of the diffusion coefficient even in the cases of total previous failure.

The obtained data are important for the proper simulation computations of diffusion processes and for the correct physical interpretation of obtained results.

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ОСОБЛИВОСТІ МОДЕЛЮВАННЯ ПРОЦЕСІВ ДИФУЗІЇ ЧАСТИНОК У ПРОСТОРОВО-ПЕРІОДИЧНИХ ПОЛЯХ

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Робота присвячена дослідженню особливостей моделювання процесів дифузії частинок у просторово-періодичних потенціалах за допомогою рівнянь Ланжевена. Проаналізовані різні методи завдання початкових умов та їхній вплив на отримані рішення. Показано, що при всіх способах завдання початкових умов система є неврівноваженою протягом деякого интервалу часу t_{trm}. Цей інтервал збільшується зі зменшенням коефіцієнту тертя як $1/\gamma$. Для адекватного опису перехідних процесів дифузії та транспорту необхідно заздалегідь проводити процедуру термалізації системи. Запропоновано новий метод завдання початкових умов, який найбільш близько описує врівноважену систему. Він полягає в генерації початкових координат та швидкостей частинок, які відповідають врівноваженому розподілу гармонійних осциляторів із даною температурою. Використання таких початкових умов дозволяє з високою точністю проводити обчислення без використання процедури термалізації при температурах $T < 0.1$. Проаналізований класичний метод визначення коефіцієнтів дифузії D як границі $\lim\limits_{t\to\infty}\left(\sigma^2/2t\right)$. Показано, що його застосування у комп’ютерних розрахунках лімітовано обмеженим часом розрахунків. Це призводить до неможливості обчислення D в деяких умовах. Запропоновано новий метод визначення коефіцієнта дифузії за лінійною апроксимацією залежності дисперсії від часу. Така апроксимація можлива тільки після того, як кінетична температура досягла свого стаціонарного значення. Запропонований метод потребує на декілька порядків менше розрахункового часу, ніж класичний метод. Внаслідок цього він дозволяє обчислювати коефіцієнт дифузії навіть у тих випадках, у яких раніше це не вдавалося. Отримані результати важливі для коректного проведення моделюючих розрахунків процесів дифузії та вірної фізичної інтерпретації отриманих результатів.

Ключові слова: дифузія, зовнішні поля, комп’ютерне моделювання, початкові умови, рівняння Ланжевена.