East Eur. J. Phys. **3**. 25-29 (2021) DOI:10.26565/2312-4334-2021-3-03

ENHANCING THE DIFFUSION IN UNDERDAMPED SPACE-PERIODIC SYSTEMS BY APPLYING EXTERNAL LOW-FREQUENCY FIELDS[†]

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Received June 11, 2021; revised July 5, 2021; accepted July 28, 2021

This paper is devoted to the studies of the opportunities for the intensification of the particle diffusion in the periodic structures, for example the crystals that are exposed to the action of the time-periodic fields of a different nature. These can be acoustic or electromagnetic fields. The trivial one-dimensional model of the motion of the particles in the potential lattice field under the thermal equilibrium has been used. The paper studies the interaction of rectangular fields with the frequencies less than 0.01 ω_0, where ω_0 is the frequency of natural small vibrations of the particles in the systems with the low dissipation. The selected friction coefficient in dimensionless units is equal to $\gamma' = 0.03$. The amplitude dependence of the intensification of the diffusion D under the action of the fields of a different frequency has been studied. It was shown that the diffusion coefficient can be increased by several orders of magnitude by applying the field of an appropriate amplitude and frequency. A maximum diffusion intensification is attained at $\omega \to 0$. A maximum attained value of the diffusion coefficient at the periodic force corresponds to the case of the action of the constant force. However, at low frequencies a maximum intensification is only possible in the narrow range of field amplitudes $F' \propto \gamma'$. A further increase in the field amplitude results in a decrease of the diffusion coefficient and it attains the value of the coefficient of the particle diffusion in the viscous medium $D_{vis} = k'T'/\gamma'$, where k' is the Boltzmann coefficient and T' is the temperature. An increase in the frequency of the external force results in the extension of the range of forces at which $D > D_{vis}$, however the value of the diffusion intensification is decreased. It was shown that the exceed of a certain threshold value of the amplitude of the external field results in the gain of the diffusion coefficient at least by the value of $\eta = (k'T'e^{\varepsilon/k'T'})/(\gamma' D_0)$, where ε is the value of the energy barrier during the passage of the particle from one cell of the one-dimensional lattice to another. The obtained data open prospects for the development of new technologies to exercise control over diffusion processes. It is of great importance for the production of nanomaterials with the specified structure, creation of the surface nanostructures, etc.
Keywords: Brownian motion, computer simulation, crystals, diffusion, Langevin equations, periodic fields, periodic systems.
PACS: 05.40.-a, 02.50.Ey, 68.43.Jk, 66.30.J-

The process of the creation of the appropriate micro- and nanostructure of the materials is reduced in many respects to the finding of an opportunity for the control over diffusion processes [1]. Up to this day, the temperature was the main parameter of such a control. The diffusion is intensified with an increase in temperature and it results in the activation of other thermal processes. From the standpoint of the technology, it is important to know how to control the diffusion of the certain types of defects or atoms without changing the medium temperature. The application of the external fields of a different nature can solve this problem on the whole.

The latest experimental investigations are indicative of that the diffusion mobility can efficiently be controlled using external fields. A huge increase in the diffusion was observed during the investigations carried out to study the motion of paramagnetic particles across the surface of garnet ferrites exposed to the action of external time-periodic magnetic fields [2]. The intensification of the diffusivity by several orders of magnitude was observed when studying the particle diffusion in the colloids with optical traps [3]. However, the physical basics of such diffusion intensification are still not very clear.

Earlier, the diffusion intensification carried out by using theoretical methods was mainly studied under the action of constant force. It was established that the diffusion mobility of the particles can essentially be increased under the action of the force both in underdamped [4] and overdamped systems [5]. It was shown in [6] that the particle diffusion coefficient can be increased in the periodic lattice by many orders of magnitude under the action of the constant external force in the narrow force range specified by the dissipative properties of the medium. The paper [7] gives analytical expressions to compute the gaining in the diffusion coefficient depending on the friction coefficient for underdamped systems. The paper [8] gives the plotted diagram of the existence of the domains that allow for the efficient control of

[†]*Cite as:* I.G. Marchenko, V.Yu. Aksenova, I.I. Marchenko, East. Eur. J. Phys. **3**, 25 (2021), https://doi.org/10.26565/2312-4334-2021-3-03

the diffusion by external constant fields. It was shown that the phenomenon of the so-called temperature-abnormal diffusion (TAD) is realized in such domains. In the case of the TAD, the diffusion coefficient is increased with the temperature drop. At first glimpse, it runs counter to our intuitive notions of diffusion processes. However, it should be noted that such a phenomenon is realized only in the systems that are far from the equilibrium.

As a rule, it is a rather complicated task to realize the conditions for the action of the constant force on a technological level. In practice, it is more promising to apply time-varying fields. Acoustic or electromagnetic fields can be used for such purpose. The authors of [9] showed that the applied periodic field can have a great effect on the diffusion coefficient in the overdamped system. The paper [10] studied diffusion processes under the action of periodic fields in underdamped systems. It was shown that considerable diffusion intensification occurs at much lower vibration amplitudes of the external field in comparison to the overdamped case. Only narrow range of the amplitudes of the periodic force was studied near a maximum value of the coefficient gain at a constant force. However, a change in the diffusion coefficient in the wide amplitude range was not studied. The main purpose of this research was to study the amplitude dependences of the diffusion intensification under the action of the external low-frequency periodic fields.

SIMULATION METHODS

The motion of Brownian particles on the one-dimensional lattice under the action of the time-periodic force $F(t)$ was described by the Langevin equation:

$$m\ddot{x} = -\frac{\partial}{\partial x}U(x) - \gamma\dot{x} + F_t(t) + \sqrt{2\gamma Q}\xi(t), \tag{1}$$

where t is the time, x is the particle coordinate, m is its mass, γ is the friction coefficient, $\xi(t)$ is the white Gaussian noise with the intensity set to unity. The point above denotes the differentiation in time. The thermal energy is $Q = kT$, where k is the Boltzmann constant and T is the temperature.

To look into physical causes for the intensified diffusion under the action of the periodic force we will consider by analogy to [10] the particle motion under the action of the rectangular periodic field.

$$F_t(t) = F sign(\sin(\omega t)) \tag{2}$$

Where ω is the angular frequency of the external force and F is its amplitude.

The given type of the external field has an advantage over the sinusoidal field from the standpoint of the simplicity of the interpretation of physical results, because under such action the particle ensemble moves in the fixed potential at each half-period. It considerably simplifies the analysis of the obtained data. The use of the sinusoidal dependence, as it was shown in [10], has no effect on the main physical results that remain unchanged and it only varies the obtained numerical values.

The potential particle energy of U in the one-dimensional lattice was equal to:

$$U(x) = -\frac{U_0}{2}\cos\left(\frac{2\pi}{a}x\right), \tag{3}$$

where a is the one-dimensional lattice period, and 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}:

$$F_{lat} = -\frac{\partial U}{\partial x} = F_0 \sin\left(\frac{2\pi}{a}x\right). \tag{4}$$

The value of $F_0 = \frac{\pi}{a}U_0$ that is called a critical force corresponds to a minimum acting force required for the overcoming of the energy barrier in the viscous medium and that energy barrier separates two neighboring positions of the particles on the one-dimensional lattice.

The parameters of the used space –periodic potential were similar to those described in [6-8], i.e. $U_0 = 0{,}08$ eV, $a = 2{,}0$ Å. The particle mass corresponded to the hydrogen mass and it was equal to 1 atomic mass unit.

The stochastic equation (1) was solved numerically for each particle with the time step less than 0.01 of the natural period of vibrations $\tau_0 = a(2m/U_0)^{1/2}$. The statistical averaging was carried out in terms of the ensemble with the particle number of at least $N = 5 \cdot 10^4$. The initial conditions were the same as in [6-8].

To analyze the simulation data it is convenient to change to non-dimensional values [11-12].

After the transformation of

$$x' = \frac{2\pi}{a}x \quad , \quad t' = \frac{y}{\tau_0} \tag{5}$$

and assuming that the non-dimensional mass $m=1$, we will obtained a maximum simple equation form (1):

$$\ddot{x}' = -\sin x' - \gamma' \dot{x}' + F'\left(t'\right) + \sqrt{2\gamma' T'}\,\zeta(t') \;, \tag{6}$$

Non-dimensional units are relating to the force, friction coefficient and the temperature as follows:

$$\gamma' = \gamma \frac{\tau_0}{2\pi m} \quad , \quad F' = \frac{F}{F_0} \qquad T' = \frac{2kT}{U_0} . \tag{7}$$

The value of $\gamma' \approx 0.032$ for the given investigation was the same as in the case of previous investigations [6-8]. The diffusion coefficient was calculated in terms of the dispersion $\sigma^2 = \left\langle \left(x' - \left\langle x' \right\rangle\right)^2 \right\rangle$ for the moving particle ensemble distribution when the time tends to the infinity:

$$D = \lim_{t \to \infty} \frac{\sigma^2}{2t} , \tag{8}$$

where the brackets $\langle ... \rangle$ denote the ensemble averaging.

To improve the computation accuracy at the limited time the diffusion coefficient was calculated in the following manner. Each computation anticipated the determination of the time t_{lin} required for the attainment of the linear dispersion-time dependence. The one-dimensional lattice diffusion coefficient was defined as ½ of the curve slope $\sigma^2(t)$. The linear dependence was obtained by the simulation data diddling using the method of least squares at the time of $t > 100 t_{lin}$. The diddling reliability was within 0.999 in all cases.

THE OBTAINED RESULTS AND DISCUSSION

Let's consider a change in the diffusion mobility of the particles under the external periodic force. To clarify the gain rate of the diffusion coefficient we calculated first the diffusion coefficients of the particles $D_{lat}\left(T'\right)$ in the absence of the external force. In Fig. 1, the dependence of $D_{lat}\left(T'\right)$ is represented by hollow markers. It has the form of the Arrenius curve that is peculiar for crystalline materials $D_{lat}\left(T'\right) = D_0 e^{-\varepsilon / kT'}$, where ε is the value of the energy barrier when the particle passes from one cell of the one-dimensional lattice to another. And the diffusion coefficient of free particles is exponentially decreased with an increase in the reciprocal temperature.

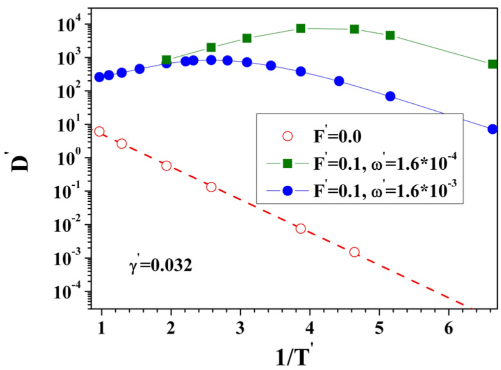

Figure 1. The dependences of diffusion coefficients on the reciprocal temperature. Empty markers denote the external force $F' = 0.0$, filled markers denote the external periodic force $F' = 0.1$ (it corresponds to a maximum diffusion coefficient at a constant force), The friction coefficient is $\gamma' = 3 \cdot 10^{-2}$. Square markers represent the frequency $\omega' = 10^{-4}$, circles indicate the frequency $\omega' = 10^{-3}$.

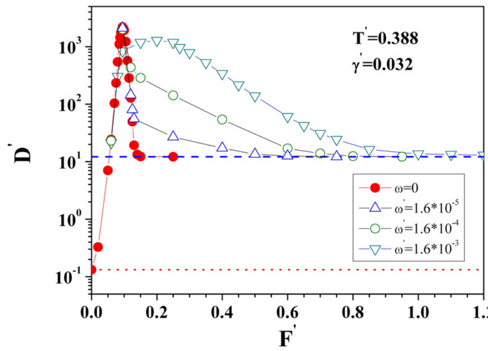

Figure 2. The dependences of diffusion coefficients on the vibration amplitude of the external periodic force F' for different frequencies of ω . The dotted line shows the value of the diffusion coefficient in the periodic lattice in the absence of the external force. The dashed line shows the value of the diffusion coefficient in the viscous unstructured medium. $T' = 0.388$, $\gamma' = 3 \cdot 10^{-2}$.

The use of the external constant field ($\omega' = 0$) results in the enhanced diffusion mobility of the particles. This gain rate depends to a great extent on the value of external force. In Fig. 2, the filled markers show the dependence of the diffusion coefficient on the value of applied force at a constant temperature of the thermostat. The dotted line in this Figure shows the value of the diffusion coefficient D_{lat} of the particles in the one –dimensional lattice in the absence of the external force. The dashed line in this Figure shows the value of the diffusion coefficient in the viscous medium of $D_{vis} = k^{'}T^{'}/\gamma^{'}$ in the absence of external forces. It can be seen that the diffusion rises sharply in the narrow range of applied forces. A maximum value of $D^{'}$ is attained at $F^{'} \approx 0.1$. Fig. 1 gives the temperature dependences of the diffusion coefficient of the particles at the same force amplitude value for the two different frequencies. The Figure shows that the application of external periodic field also increases the diffusion mobility of the particles by several orders of magnitude in the wide temperature range. Moreover, the diffusion coefficient is increased in the specified temperature range with the temperature drop. It is the range of the so-called temperature – abnormal diffusion. By decreasing the external force frequency we extend this temperature range. In other words, by changing the external force frequency we can efficiently control the diffusion coefficient at the given temperature.

Let's consider in detail a change in the dependence of the diffusion coefficient on the amplitude of external vibrations for different frequencies of the external force. Fig. 2 shows such dependencies for the fixed temperature of $T^{'} = 0.388$. It can be seen that for the frequency range in question, $D^{'}$ is always increased from the value of D_{lat}, attaining a certain maximum value of $D_{\max}$, and then it drops to the value of D_{vis}. A further increase in the amplitude results in no change of the diffusion coefficient. It means that in the case of exceed of a certain critical amplitude value we observe the gain in the diffusion coefficient as a minimum by the value of $\eta = D_{vis}/D_{lat} = \dfrac{k^{'}T^{'}e^{\varepsilon/k^{'}T^{'}}}{\gamma^{'}D_0}$.

The highest diffusion intensification is observed at low frequencies. At the frequency of $\omega^{'} = 1.6*10^{-5}$, the curve of $D^{'}\left(F^{'};\omega^{'}\right)$ coincides with the curve of a change in the diffusion coefficient under the action of the static force $F^{'} \le 0.13$. It is well-known [12] that the so-called running and locked solutions can exist simultaneously in underdamped periodic systems. It was shown earlier [13] that an increase in the diffusion coefficient under the action of the constant force occurs due to the appearance of the localized and moving particles in the ensemble of the "populations" particles under the action of the thermal noise. The solution of equation (1) with no random force showed that running stationary solutions are unavailable in studied frequency and amplitude ranges. At each half-period, the particles change to the moving state and make long jumps. Afterwards, these are returned to the localized state and begin their motion from new nodes. As a matter of fact, the diffusion is intensified.

A specific feature of the low-frequency vibrations of a low amplitude is that the particle velocity distributions of $n\left(V^{'}\right)$ coincide during the half-period for constant and periodic forces. Therefore, at low frequencies ($\omega^{'} = 1.6*10^{-5}$) up to the values of $F^{'} \approx 0.13$ the curve of $D^{'}\left(F^{'}\right)$ coincides with the curve for the case of $\omega = 0$. At high amplitude values, the diffusion coefficient scarcely differs from D_{vis}. The increase in the frequency up to the value of $\omega^{'} = 1.6*10^{-4}$ provides a noticeable difference of the diffusion coefficient in contrast to $D^{'}\left(F^{'};\omega = 0\right)$ at $F^{'} > 0.12$. At the frequencies above $\omega^{'} > 1.6*10^{-3}$ the diffusion coefficient of $D(\omega)$ fails to attain the value of $D_{\max}$ and it considerably differs from $D^{'}\left(F^{'};0\right)$. In other words, a certain specific frequency range exists and it permits maximum diffusion intensification by varying the amplitude of external vibrations. At the same time, the amplitude range in which $D^{/}\left(\omega^{'}\right) > D_{vis}$ is extended with an increase in frequency. In this case, the curve maximum $D^{'}\left(F^{'};\omega\right)$ is shifted towards the range of higher amplitudes.

Hence, we showed that the action of the periodic field always results in the enhancement of diffusion processes. A maximum intensification is observed al low frequencies in the narrow amplitude range. An increase in the frequency extends the intensified diffusion domain. It is related to the fact that the diffusion intensification mechanism differs in the case of constant and periodic fields. In the case of the constant field, the diffusion coefficient is defined by the stationary particle distribution between the two ensembles, in particular, the "running" and "localized" states. In the case of the action of the periodic field throughout the period the particle velocity distribution function is changed all the time [14].

CONCLUSIONS

This paper delves into the studies of the intensification of the particle diffusion in the one-dimensional space lattice exposed to the action of the external low-frequency time-periodic fields. It was shown that the diffusion coefficient can be increased by several orders of magnitude by applying the field of an appropriate amplitude and frequency. A maximum diffusion intensification is observed at $\omega \to 0$. For the studied frequency range we can state that the diffusion coefficient tends to the diffusion coefficient in the viscous medium at increased force amplitudes. The obtained data open prospects for the development of new technologies to exercise control over diffusion processes. It is of great importance for the production of nanomaterials with the specified structure, creation of the surface nanostructures, etc.

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ПОСИЛЕННЯ ДИФУЗІЇ В НЕДОДЕМПФОВАНИХ ПРОСТОРОВО-ПЕРІОДИЧНИХ СИСТЕМАХ ЗОВНІШНІМИ НИЗЬКОЧАСТОТНИМИ ПОЛЯМИ

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Робота присвячена дослідженню можливості посилення дифузії частинок в періодичних структурах, таких як кристали, за допомогою впливу на них зовнішніми періодичними в часі полями різної природи. В якості таких можуть виступати акустичні або електромагнітні поля. Використана найпростіша одномірна модель руху частинок, що знаходяться в потенційному полі решітці та в тепловій рівновазі з термостатом. В роботі вивчено вплив прямокутного поля з частотами менше 0.01 ω_0, де ω_0 – частота власних малих коливань частинок у системах із малою дисипацією. Обраний коефіцієнт тертя в безрозмірних одиницях дорівнював $\gamma' = 0.03$. Вивчена амплітудна залежність посилення дифузії D під впливом полів різної частоти. Показано, що коефіцієнт дифузії може бути посилений на кілька порядків із застосуванням поля відповідної амплітуди і частоти. Найбільше посилення дифузії досягається при $\omega \to 0$. Максимально досяжне значення коефіцієнта дифузії при періодичному впливі відповідає випадку впливу постійної сили. Однак при низьких частотах максимальне посилення можливо тільки у вузькому діапазоні амплітуд поля $F' \propto \gamma'$. При подальшому збільшенні амплітуди поля коефіцієнт дифузії зменшується та досягає величини коефіцієнта дифузії частинок у в'язкому середовищі $D_{vis} = k'T'/\gamma'$, де k' – коефіцієнт Больцмана, а T' – температура. Збільшення частоти зовнішнього впливу призводить до розширення інтервалу сил, при яких $D > D_{vis}$, однак величина посилення дифузії зменшується. Показано, що при перевищенні деякого порогового значення амплітуди зовнішнього поля спостерігається посилення коефіцієнта дифузії як мінімум на значення $\eta = (k'T'e^{\varepsilon/k'T'})/(\gamma' D_0)$, де ε – величина енергетичного бар'єра при переході частинки з однієї комірки одновимірної решітки в іншу. Отримані результати відкривають перспективи створення нових технологій управління процесами дифузії. Це має велике значення для отримання наноматеріалів із заданою структурою, створення поверхневих наноструктур і т.п.

Ключові слова: броунівський рух, дифузія, комп'ютерне моделювання, кристали, періодичні поля, рівняння Ланжевена.