COMPUTER SIMULATION OF DIFFUSIVITY – TEMPERATURE BEHAVIOR IN DRIVEN PERIODIC SYSTEMS

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We investigate how the temperature dependence of diffusion changes with varying friction in spatially periodic systems driven by an external high-frequency field. Our results show that, depending on the system’s parameters, diffusion can either grow or decay exponentially with inverse temperature — and in some cases, remain almost constant across specific temperature ranges. This rich variety of behaviors is analyzed in the context of the stability of localized and transport attractors under thermal fluctuations.

Diffusion-limited processes are fundamental in physics, chemistry, biology, and other fields of natural science. The temperature dependence of the diffusion coefficient D often plays a crucial role in determining the dynamics of such processes. In unstructured media, diffusion typically increases linearly with temperature, D~Q, where Q denotes the thermal noise intensity [1, 2]. When particles move in spatially periodic structures, the functional form of D(T) can significantly change. Two limiting cases are usually distinguished: the overdamped regime ($\gamma \gg 1$) and the underdamped regime ($\gamma \ll 1$). For a simple one-dimensional cosine potential, analytical expressions for the diffusion coefficient have been obtained in both limits. In the high-temperature limit, the diffusion scales linearly with noise intensity, D~Q [3]. In contrast, in the low-temperature regime, it follows an Arrhenius-like exponential decay, D~exp(-e/Q), where e is the amplitude of the periodic potential [4].

Under nonequilibrium conditions, these dependencies can change dramatically. In overdamped systems with tilted periodic potentials, the ratio D/D_0, where D_0 is the free diffusion coefficient in a viscous medium, may increase as temperature decreases [5]. In underdamped systems, counterintuitive behavior can emerge, where the diffusion coefficient itself grows as the temperature drops [6, 7].

When the system is driven by low-frequency periodic forces, non-monotonic temperature dependence of diffusion may arise in the underdamped regime [8]. The influence of high-frequency driving was initially studied by Borromeo in overdamped systems [9], where an averaging approach over the fast oscillations – known as the vibrational mechanics framework – can be employed for large γ. In the absence of a constant bias, this approximation results in an effective periodic potential with the same spatial period but a renormalized amplitude scaled by the zeroth-order Bessel function $J_0(\psi_0)$, where ψ_0 depends on the amplitude and frequency of the external field. At the zeros of $J_0(\psi_0)$ the effective potential vanishes, and the system behaves as if it were structureless, leading to maximum possible diffusion within this model.

However, later studies revealed that in underdamped systems, diffusion can be significantly enhanced beyond this limit [10]. Moreover, the temperature dependence of diffusion becomes non-monotonic and may increase as temperature decreases.

In this work, we explore how the temperature dependence of diffusion changes under high-frequency external driving as a function of the system’s dissipation. We aim to clarify the fundamental differences between the overdamped and underdamped regimes. We demonstrate that depending on the friction coefficient, diffusion may either exponentially decrease or increase with decreasing temperature.

1. SIMULATION METHODOLOGY

To describe the motion of Brownian particles moving in a spatially periodic structure and subjected to a time-periodic force f = a sin(ωt), we used the Langevin equation in dimensionless form

$$\ddot{x} = -\sin x - \gamma\dot{x} + a\sin(\omega t) + \sqrt{2\gamma Q}\,\xi(t)\,, \qquad (1)$$

where the dot denotes differentiation with respect to time t. Here, x is the particle coordinate, a is the amplitude, and ω is the frequency of the external oscillations. In this work, we investigate the high-frequency case with a fixed external frequency ω = 1.59, which is higher than the frequency of small natural oscillations.

The parameter γ is the friction coefficient, and $Q \propto k_B T$ is the dimensionless temperature of the system. The interaction with the thermostat is modeled by δ-correlated Gaussian white noise ξ(t), with $\langle\xi(t)\rangle = 0$ and $\langle\xi(t)\xi(s)\rangle = \delta(t-s)$. Note that in this scaling, the dimensionless mass m = 1.

The Langevin equation was integrated using the Heun method with a time step of less than 0.01 of the natural period. Statistical averaging was performed over an ensemble of no fewer than $N = 5\cdot10^4$ particles. Initial conditions were as follows: particle coordinates x(0) were uniformly distributed over the interval [0, 2π], and velocities v(0) over the interval [−2, 2].

All calculations were carried out using a Compute Unified Device Architecture (CUDA) implemented on a modern GPU, providing approximately 1000x speed-up compared to CPU computation.

To calculate the diffusion coefficient, we used a method based on calculating the dispersion σ^2 of the distribution of an ensemble of particles as time approaches infinity:

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

To analyze particle motion, including thermally activated and deterministic regimes, we used the period-averaged velocity:

$$V(t)=\tfrac{1}{\tau}\int_{t}^{t+\tau}\dot{x}(s)\,ds \qquad (3)$$

to classify particles by attractor type.

For analyzing attractor stability in the deterministic case ($Q \equiv 0$), we computed Lyapunov exponents using the Benettin algorithm [11], integrating both the nonlinear motion equations and variational equations. Gram-Schmidt orthonormalization was applied at adaptive intervals to maintain vector independence.

2. TEMPERATURE DEPENDENCE OF DIFFUSION FOR DIFFERENT VALUES OF FRICTION COEFFICIENT

To understand how the temperature dependence of diffusion varies with changing friction, we first examine the amplitude dependence of the diffusion coefficient for three characteristic values of the friction coefficient. These values correspond to the overdamped case (γ=3), the underdamped case (γ=0.03), and an intermediate damping regime (γ=0.3). Figure 1 presents the diffusion coefficient as a function of the driving amplitude for two different values of the thermal noise intensity: Q=0.5 and Q=0.1. For both temperatures, as previously reported [10], the diffusion exhibits a quasiperiodic dependence on the driving amplitude. As γ increases, the locations of the extrema shift toward higher amplitudes.

Notably, the temperature dependence of diffusion at these extrema differs qualitatively with varying γ. In the minima of the diffusion–amplitude curves, lower temperatures consistently yield smaller diffusion coefficients. However, at the maxima of D(a), the behavior of D(Q) qualitatively changes with γ. Specifically, for γ=3, we find D(0.5)>D(0.1); for γ=0.3 D(0.5)≈D(0.1); and for γ=0.03, the relation reverses, with D(0.5)<D(0.1).

As shown previously, in the overdamped regime, the amplitude dependence of the diffusion coefficient is well captured by the vibrational mechanics method. Within this framework, the positions of the extrema are independent of temperature. However, as seen in Fig. 1,b, the first maximum at Q=0.1 (marked as point 3) is shifted relative to the corresponding maximum at Q=0.5, indicating that this approximation becomes less accurate in some regimes.

Therefore, for the remainder of our analysis, we use the amplitude values corresponding to the extrema of D(a) at the lower temperature Q=0.1. In Fig. 1, points labeled 1, 3, and 5 denote the amplitudes at which diffusion reaches a maximum for different values of γ, while points labeled 2, 4, and 6 correspond to the amplitudes where diffusion attains a minimum.

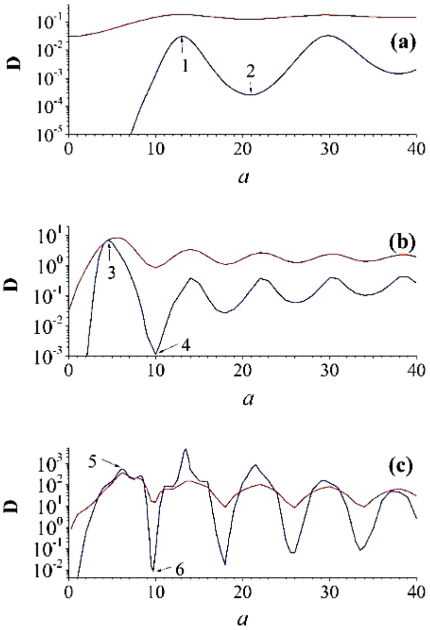

Fig. 1. Diffusion coefficient as a function of external force amplitude for different friction coefficients at two different temperatures.
T=0.5 – red curve; T=0.1 – blue curve.
a – ɣ=3.0; b – ɣ=0.3; c – ɣ=0.03. Numbers indicate the positions of the first diffusion maxima and minima for different ɣ

Fig. 2 presents the temperature dependence D(Q) for the amplitudes marked in Fig. 1 by points 1, 3, and 5. These correspond to three distinct physical regimes: (1) the overdamped system (γ=3.0), (3) moderate damping (γ=0.3), and (5) the underdamped system (γ=0.03). As seen in the figure, the character of the temperature dependence changes qualitatively with friction. For strong damping, the diffusion coefficient D increases linearly with temperature. This behavior is consistent with diffusion in a structureless viscous medium. In contrast, in the underdamped regime, we observe anomalous diffusion where $\partial D/\partial Q<0$, and the diffusion coefficient diverges exponentially as temperature approaches zero: D→∞ as T→0. Finally, for the intermediate damping (γ=0.3), the diffusion remains nearly constant over a wide temperature range 0.05<Q<1.0.

To understand the origin of these behaviors, we examine the inset in Fig. 2, which shows the period-averaged velocity distributions n(V) at a low temperature Q=0.05. This temperature level is indicated by a vertical dashed line in the main panel. The distinction between the overdamped and underdamped cases is immediately apparent. While n(V) exhibits three local maxima for γ=0.3 and five for γ=0.03, the overdamped case γ=3.0 shows only a single peak.

A Lyapunov stability analysis confirms that the overdamped system supports only localized attractors. In the presence of thermal noise, this leads to a unimodal velocity distribution centered at V=0, as seen for γ=3.0.

As shown previously, the amplitude dependence of the diffusion coefficient in strongly damped systems at fixed temperature is well captured by the vibrational mechanics model. This approach, based on Kapitza's averaged field method, treats particle motion in a spatially periodic potential under a high-frequency external field as motion in an effective time-averaged periodic potential. The diffusion maximum D(a) occurs when the amplitude of this effective potential vanishes. Thus, at amplitudes corresponding to local maxima of diffusion, particle motion resembles random diffusion in a structureless viscous medium. The blue curve (labeled 1) in Fig. 2 illustrates that in this case, diffusion increases linearly with temperature ($D \sim Q$), in agreement with the predictions of vibrational mechanics.

However, the case of low damping (see curve 5) cannot be explained within this model. First, because diffusion increases as temperature decreases – contrary to the model's predictions – and second, because the maximum attainable value of D in the vibrational mechanics framework cannot exceed Q/γ.

As demonstrated in Ref. [10], underdamped deterministic systems can exhibit transport attractors. A stability analysis shows that for $\gamma=0.03$ and $a=6.0$, the deterministic system supports not only localized solutions but also Lyapunov-stable running solutions. The largest Lyapunov exponent for all attractors was approximately $\lambda \approx -0.015$. In the presence of thermal noise, transitions occur between different attractors, resulting in a stationary velocity distribution n(V). The inset in Fig. 2 shows this distribution (red curve) for $\gamma=0.03$, which is qualitatively different from that for $\gamma=3.0$. While the overdamped case yields a single peak near $V=0$, the underdamped regime displays pronounced peaks at $V/\omega=\pm 1$ and $V/\omega=\pm 2$. Notably, the heights of the peaks corresponding to the transport attractors at $V/\omega=\pm 1$ are comparable to that of the localized attractor, highlighting the significant role of running states in the system's dynamics. Existence of particle populations with average velocities $V/\omega=\pm 1$ determines the temperature dependence of diffusion in the underdamped regime

The green curve in the inset of Fig. 2 shows the distribution of average velocities for the case of $\gamma=0.3$. The presence of particles at $V=0$ and $V/\omega=\pm 1$ is clearly visible, but the majority are localized around $V=0$. Unlike in the underdamped regime, particles with $V/\omega=\pm 2$ are not present. The function n(V) depends on temperature, but as the temperature decreases, it converges to a stationary distribution. At high temperatures, the diffusion behavior follows the standard expression $D = \frac{Q}{\gamma}$, and the influence of the periodic potential becomes negligible.

We apply the vibrational mechanics method to calculate diffusion in the overdamped regime. In Fig. 3, the results of this calculation are shown with a blue dashed line. It can be seen that in the high-friction case, the analytical predictions match the simulation data across the entire temperature range. At low temperatures, the asymptotic dependence $D \sim \exp(-\beta/Q)$ holds, and for $Q \gg 1$ $D \to Q/\gamma$. Thus, for the overdamped case, the vibrational mechanics model accurately describes diffusion both at the maximum and at the minimum of D(a).

A different picture is observed for the low-friction case. In Fig. 3, red circular markers show the diffusion data for small damping. As can be seen from the graph, at low temperatures the dependence is well approximated $D \sim \exp(-\beta/Q)$. This qualitatively agrees with the vibrational mechanics model. However, this behavior sharply contrasts with the temperature dependence of diffusion at the maximum of D(a) for low damping (see Fig. 2). The reason lies in the fact that at the local minimum of diffusion, only localized attractors remain stable at low temperatures. This is clearly seen in the bottom inset of Fig. 3, which shows the distribution of particle velocities V. It is evident that the ensemble contains only particles with $V=0$. In this case, the key assumption of the effective potential theory – small particle displacement over one period of the external force – holds true. Therefore, the observed decrease in diffusion is well captured by the vibrational mechanics model.

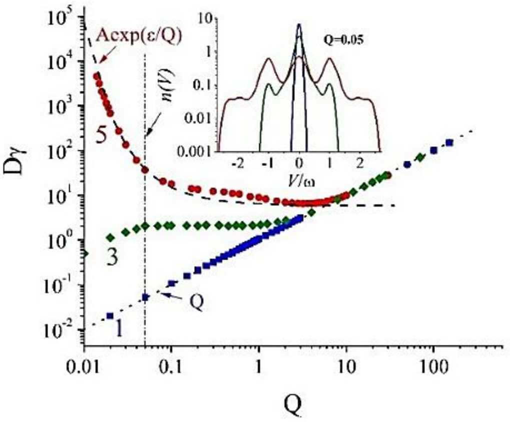

Fig. 2. Temperature dependence of $D\gamma$ at points 1, 3, and 5 in Fig. 1 (first maximum of the amplitude dependence). 1 – $\gamma=3.0$, $a=13$; 3 – $\gamma=0.3$, $a=4.5$; 5 – $\gamma=0.03$, $a=6.0$. The dashed line represents the exponential dependence with $\mathcal{E}=0.09436$. The dotted line represents the linear dependence.
Insert – Distribution functions for the average velocities over the period for three graphs at $Q=0.05$ (marked by the dotted line in the main figure

At the same time, at $Q \equiv 0$ for $\gamma=3$ and $a=9.71$, along with localized solutions, stable running solutions also exist. In the top inset, the distribution over attractors is shown in the form of a histogram. The majority (0.87) of all solutions correspond to localized attractors with $V=0$. However, there are also running solutions with $V/\omega = \pm 1, \pm 2, \pm 3, \pm 4$. All of these solutions are Lyapunov stable, with the maximum Lyapunov exponent for all such attractors approximately $\lambda \approx -0.015$. However, even a small amount of thermal noise leads to their global instability and disappearance. Thus, unlike the case of the maximum of D(a), where the population of running particles persisted as the noise decreased, in the minimum of D(a), even small noise causes the running attractors to disappear.

Generally, noise plays a destructive role and destroys attractors. However, as shown in the top inset of Fig. 3, increasing temperature leads to the appearance of populations of running particles that were absent at lower temperatures.

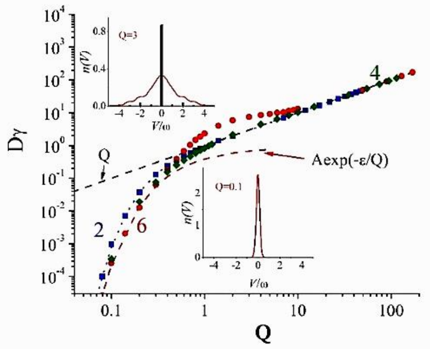

Fig. 3. Temperature dependence of Dɣ at points 2, 4, and 6 in Fig. 1. 2 – ɣ=3.0, a=20.7; 4 – ɣ=0.3, a=9.9; 6 – ɣ=0.03, a=9.71. The blue dotted line shows the D~Q dependence. The insets show the distribution functions for the average velocities over the period for three graphs at Q=0.1 and Q=3.0. The top inset in black shows the histogram of the particle distribution by V at Q=0

We clearly observe the emergence of particles with V/ω = ±1, ±2, ±3, which existed in the deterministic case. The appearance of particles with such average velocities leads to diffusion exceeding the baseline level D_0 in the range $0.6<Q<10$. Thus, in this case, the increase in the diffusion coefficient is associated with thermally activated running attractors.

CONCLUSIONS

The study conducted shows that the temperature dependence of diffusion in spatially periodic systems under the influence of a high-frequency external field can change dramatically with variations in the system’s dissipative properties. In the low-temperature limit, one can observe both exponential decrease and exponential increase of diffusion with decreasing temperature. Diffusion enhancement can also be observed at temperatures an order of magnitude higher than the energy barrier of the spatial lattice.

All of these features are determined by the behavior of attractors under the influence of thermal noise. Noise, in this context, can either enhance or suppress diffusion.

Typically, particle dynamics are described based on the attractors of the deterministic system. Their local stability is characterized by Lyapunov exponents λ, which are relatively easy to compute because they depend only on the equations of motion linearized around the steady-state solution. At the same time, global stability measures, which depend on the full nonlinear response of the system, are generally much harder to evaluate, and the information they provide can paint a qualitatively different picture than local stability metrics.

As our study shows, the dynamics of a Brownian particle ensemble are governed primarily by the global stability of attractors, which can differ from their linear stability. Moreover, some attractors become unstable even under weak noise, while others may be activated by sufficiently strong thermal noise.

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КОМП'ЮТЕРНЕ МОДЕЛЮВАННЯ ЗАЛЕЖНОСТІ ДИФУЗІЇ ВІД ТЕМПЕРАТУРИ У ЗОВНІШНЬО ЗБУРЕНИХ ПЕРІОДИЧНИХ СИСТЕМАХ

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Ми досліджуємо, як змінюється температурна залежність дифузії з різним тертям у просторово-періодичних системах, що керуються зовнішнім високочастотним полем. Наші результати показують, що залежно від параметрів системи, дифузія може або зростати, або згасати експоненціально з оберненою температурою, а в деяких випадках залишатися майже постійною в певних температурних діапазонах. Це багате розмаїття поведінки аналізується в контексті стабільності локалізованих та транспортних атракторів за теплових коливань.