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Non-Stationary and Resonant Passage of a System: A High-Frequency Cutoff Noise

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Abstract

We study non-equilibrium behaviors of a particle subjected to a high-frequency cutoff noise in terms of generalized Langevin equation, where the spectrum of internal noise is considered to be of the generalized Debye form. A closed solution is impossible even if the equation is linear, because the Laplace transform of the memory kernel is a multi-value function. We use a numerical method to calculate the velocity correlation function of a force-free particle and the probability of a particle passing over the top of an inverse harmonic potential. We indicate the nonergodicity of the second type, *i.e.*, the auto-correlation function of the velocity approaches to non-stationary at large times. Applied to the barrier passage problem, we find and analyse a resonant phenomenon that the dependence of the cutoff frequency is nonmonotonic when the initial directional velocity of the particle is less than the critical value, the latter is determined by the passing probability equal to 0.5.

Keywords

Nonergodicity, Generalized Debye Noise, Resonance Passing

1. Introduction and Model

The well-known Debye spectrum of noise is a common expression to study dynamic characteristics of lattices in solid physics [1] [2]. It has been successful to solve incoherent scattering cross section in [3], vibrational relaxation of impurities in solids [4] and the dynamics of glasses and liquids [5] [6]. Besides, many chemical reactions can be modeled by a single coordinate buffered by the random force and corresponding to the memory friction, both obeying the fluctuation-dissipation theorem. Starting out from the system-plus-reservoir model, this dynamics can conveniently be described by a generalized Langevin equation (GLE) [7] [8] of Mori-Lee form:

$$m\frac{\mathrm{d}}{\mathrm{d}t}v(t)+m\int_0^t\gamma(t-t')v(t')\mathrm{d}t'+\frac{\mathrm{d}U(x)}{\mathrm{d}x}=\varepsilon(t), \quad (1)$$

where the zero-mean noise $\varepsilon(t)$ obeys a Gaussian distribution and the memory kernel $\Gamma(t)$ is related to the internal noise $\varepsilon(t)$ through $\langle\varepsilon(t)\varepsilon(t')\rangle = mk_BT\gamma(t-t')$ [9]. k_B is the Boltzmann constant, T denotes the bath temperature and $U(x)$ is the external potential. The motion of the particle is affected by dissipative influence of a disordered medium. The non-Ohmic model can be described by a rich variety of frequency-dependent friction mechanisms [10], which arises from the spectral density $J(\omega)$ [11]. The relationship can be described as $\gamma(t)=\frac{1}{m}\int_0^\infty \mathrm{d}\omega\frac{J(\omega)}{\omega}\cos(\omega t)$.

The truncated form of spectral density of noise is usually chosen to be low-frequency [12] or with channel-frequency cutoff [13] [14]. If the spectrum of noise is replaced by the generalized Debye form, non-equilibrium properties, the fundamental variables and other properties in a such thermal fluctuation environment can be further obtained. Moreover, the non-equilibrium characteristics in such system are investigated, but its dynamic motions still remain open. In the present work, the environment spectrum $J(\omega)$ takes the generalized Debye form.

$$J(\omega)=\begin{cases} m\gamma_\delta\omega(\omega/\tilde{\omega})^{\delta-1}, & \omega<\omega_s \\ 0, & \omega>\omega_s \end{cases} \quad (2)$$

This corresponds, e.g., to the long-wavelength limit of one-dimensional acoustic phonons. For a noise originated from a coupled oscillator chain, ω_s is the Debye phonon frequency, $\tilde{\omega}$ denotes a reference frequency allowing for the friction to have the dimension of a viscosity of any δ. The mean square displacement of a force-free particle in the non-Ohmic thermal bath is proportional to the fractional power of the time at long times, namely, $\langle x^2(t)\rangle \propto t^\delta$. The cases of $0<\delta<1$ and $1<\delta<2$ are sub-Ohmic and super-Ohmic baths, which result in sub-diffusion and super-diffusion, respectively; $\delta=1$ is the Ohmic damping leading to the normal diffusion.

In this work, we pay attention to the nonergodicity of second type, which manifests that the auto-correlation function of the velocity approaches non-stationarity at large times and its dynamical effect. The paper is organized as follows. In Sec. II, we describe our GLE model subjected to a high-frequency cutoff noise. In Sec. III, the velocity auto-correlation functions of a force-free particle and a harmonic particle are calculated numerically, respectively. In Sec. IV, we address a barrier-passage problem and show a resonant phenomenon. The summary is given in Sec. V.

2. Nonergodicity of the Second Type

Within the GLE dynamics, the criterion of non-ergodicity is that the velocity autocorrelation function $C_v(t)=\langle v(t)v(0)\rangle$ of a force-free particle does not vanish in the long-time limit. In the calculations, in order to make the particle having enough time to reach equilibrium, $C_v(t)$ is calculated after $t=100$. In the following, the natural units $m=1$ and $k_B=1$, the dimensionless damping coefficient $\gamma_\delta=1.0$, as well as the time step $\Delta t=0.01$ are used. The statistic averaging is performed over the ensemble consisting of 5×10^4 particles. The test particles start from zero and their velocities are sampled from the Gaussian distribution with zero mean and width $\langle v^2(0)\rangle = k_B T/m$.

For such a finite spectrum, the physical dynamic properties of the particle in the free filed $U(x)=0$ need to be studied first. In **Figure 1**, we present the velocity correlation function obtained for subdiffusion ($\delta=0.5$), normal diffusion ($\delta=1.0$), and superdiffusion ($\delta=1.5$) for various ω_s. This measures the importance of the nonequilibrium of the system, which causes $C_v(t)$ to oscillate over the time for large t. Also, the behaviour of the oscillation of $C_v(t)$ strongly depends on the values of the Debye phonon frequency ω_s. Due to the absence of the high frequency, the energy exchange between particles and the environment is not sufficient. Thus the system can not reach to the equilibrium in the long time limit. If the frequency cutoff ω_s is small, the lower frequency cutoff of the system becomes weaker. It is conducive to the particle to dissipate kinetic energy. On the other hand, if the frequency cut ω_s is large, the damping becomes bigger. Thus the energy dissipation of the particle is increased and the energy exchange between particles and the environment becomes larger. Thus the oscillation of $C_v(t)$ is weaker when increasing the frequency cutoff.

Meanwhile, it is worth pointing out that this phenomenon of nonequilibrium is divided by the diffusion index δ, which indicates how fast the diffusion occurs. We show the relationship of $C_v(t)$ with δ in detail in **Figure 2** when

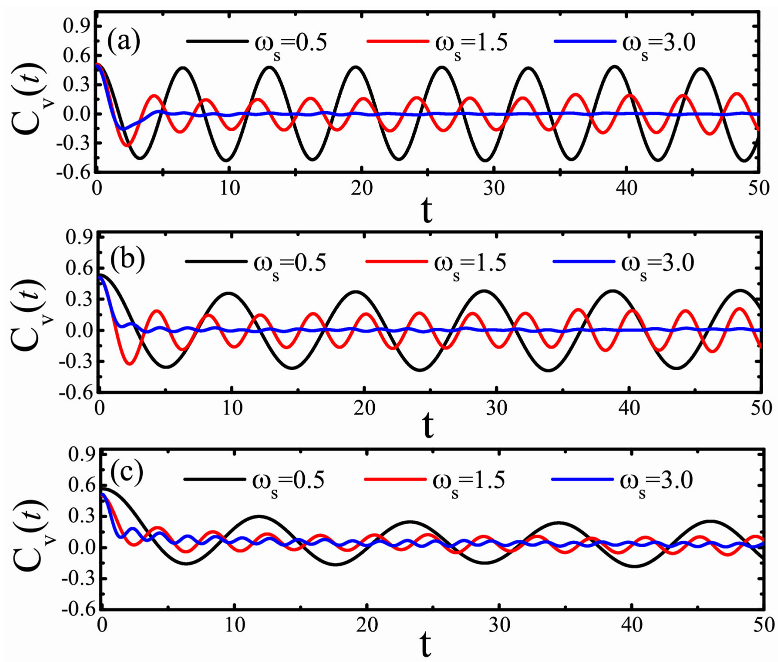

Figure 1. $C_v(t)$ as a function of time t for various ω_s at $T=0.5$. The parameters used are (a) $\delta=0.5$; (b) $\delta=1.0$; (c) $\delta=1.5$, respectively.

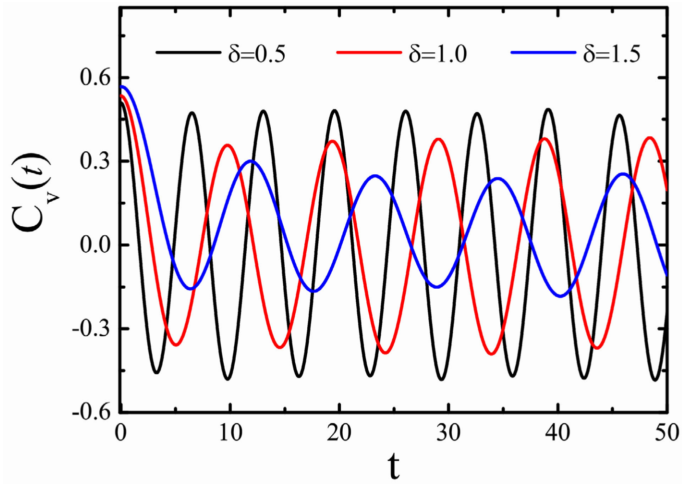

Figure 2. $C_v(t)$ as a function of time t for various δ at $T = 0.5$, $\omega_s = 0.5$.

frequency cut is small. It is seen that the amplitude of oscillation of $C_v(t)$ becomes weaker when the diffusion is strong. Namely, faster diffusion results in the non-equilibrium of the system being not obvious. As δ decreases, the particle's memory of initial state gradually increases. The fast diffusion of the particles compensates the lack of systematic dissipation. As a consequence, slow diffusion makes it harder for the system to achieve equilibrium.

For a general potential, the system will reach thermal equilibrium where the single oscillator is coupled to a finite bath of the harmonic oscillator [15]. What will happen if the particle is found in a harmonic oscillator potential $U(x) = m\omega_0^2 x^2/2$ with Debye spectrum? Can the system reach thermal equilibrium at large t? In **Figure 3**, the velocity correlation function of the particle in a harmonic oscillator potential is presented. Obviously, the oscillation behavior is weaker when the frequency of the harmonic oscillator potential ω_0 increases. But it can not reach to the thermal equilibrium considering the effects of the external harmonic oscillator potential. Ref. [16] also revealed similar effects of the harmonic potential. It is demonstrated that non-equilibration emerges because of the formation of bound states in the coupled system-plus-bath using the microscopic model of a bath as a collection of oscillator.

We now investigate nonergodicity of the second kind of a harmonic particle subjected to an internal colored noise with generalized Debye spectrum, namely, the asymptotical result of a dynamical variable does not approach a constant. The mean energy of the particle is determined by

$$\langle E(t)\rangle = \frac{1}{2} m \langle v^2(t)\rangle + \langle U(x)\rangle. \tag{3}$$

The results are plotted in **Figure 4**, where the initial variance displacement width $\langle x^2(0)\rangle$ and the initial velocity width $\langle v^2(0)\rangle$ are chosen to be $\frac{k_B}{m\omega_0^2}T_0$ and $\frac{k_B}{m}T_0$, respectively. Here, T_0 is the initial temperature of such a system. As we

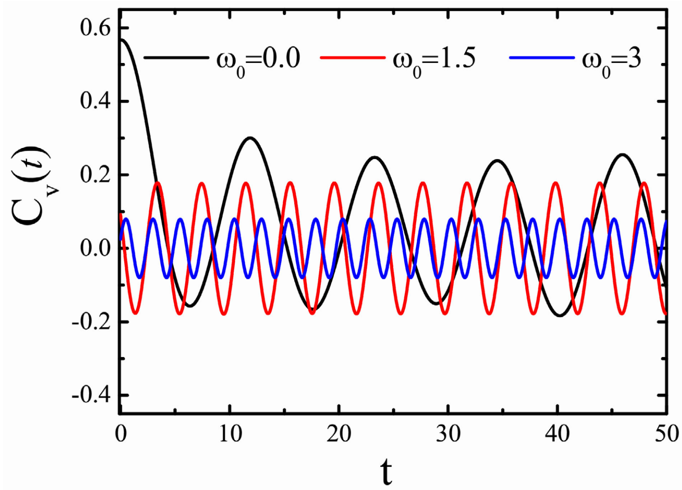

Figure 3. Time-dependent $C_v(t)$ for various frequency ω_0 in a harmonic potential. The parameters used are $T = 0.5$, $\omega_s = 0.5$, and $\delta = 1.5$.

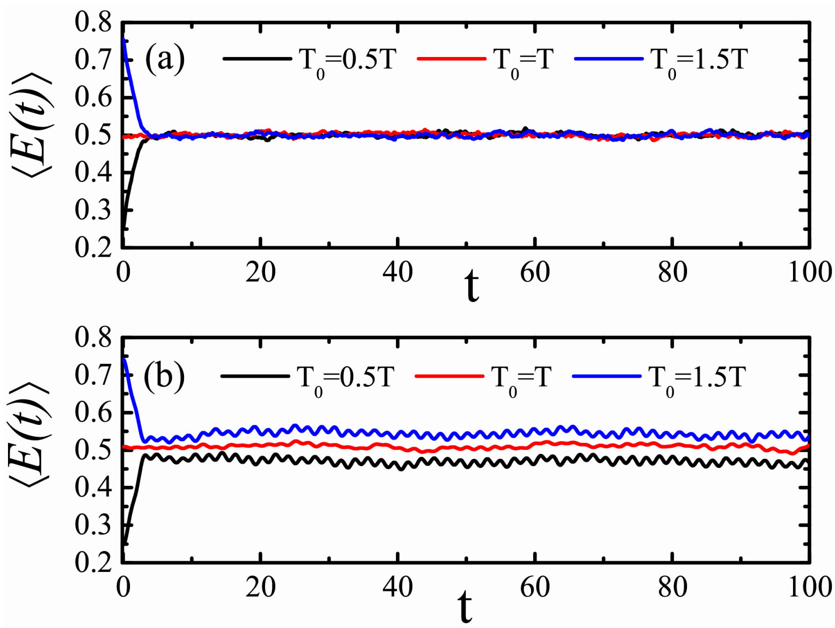

Figure 4. Time dependence mean energy $\langle E(t) \rangle$ of a harmonic particle for various initial temperatures T_0, the continuous and Debye spectrums, respectively. The parameters used are $T = 0.5$, $\omega_0 = 1.0$, $\omega_s = 1.5$, and $\delta = 1.0$.

know, in the case of a continuous spectrum, the velocities fluctuations in harmonic potential are clearly ergodic. The property of ergodicity under the condition of a continuous spectrum with the high frequency function $e^{-\omega/\omega_c}$ [17] is shown in **Figure 4(a)**. Nevertheless, as can be seen from **Figure 4(b)**, it provides a clear indication of nonergodicity of the second type in the case of a Debye spectrum. Namely, the value of $\langle E(t) \rangle$ strongly depends on the initial preparation of the particle in the limit of large times [18] [19]. Another distinct feature is revealed that the mean energy of the particle in such a system oscillates around a fixed value in the limit of time, which has the similar behaviour as already mentioned above. The stationary state can not arrive at the equilibrium one in a large time limit due to the fact of insufficient dissipation.

3. The Barrier-Passing Probability

For the barrier passage process, the potential $U(x)$ around the saddle point is treated to be an inverted parabola $-m\omega_b^2 x^2/2$. The coefficients are supposed to be constant around the saddle. Here, we define a Langevin trajectory starting from $x(t=0)=x_0$, finally crossing the saddle point $x_b=0$. Given a set of initial conditions, $x_0<0$ and $m\ddot{x}_0>0$, the Langevin equation can be exactly solved, see Refs [20] [21], and leads necessarily to a Gaussian distribution. The time-dependent passing probability is simply given by [22]

$$P(x_0,v_0,t)=\frac{1}{2}\operatorname{erfc}\left(-\frac{\langle x(t)\rangle}{\sqrt{2\sigma_x^2(t)}}\right), \tag{4}$$

where $\langle x(t)\rangle$ and $\sigma_x^2(t)$ are average position and variance of the particle and are given by

$$\langle x(t)\rangle=\left[1+\omega_b^2\int_0^t\phi_\delta(t')\mathrm{d}t'\right]x_0+\phi_\delta(t)v_0, \tag{5}$$

and

$$\sigma_x^2(t)=2mk_BT\int_0^t\mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\phi_\delta(t-t_1)\phi_\delta(t-t_2)\gamma(t_1-t_2), \tag{6}$$

respectively. The response function ϕ_δ results from its Laplace transfrom $\hat{\phi}_\delta(z)$ given by $\hat{\phi}_\delta(z)=\left[z^2+z\hat{\gamma}(z)-\omega_b^2\right]^{-1}$, in which $\gamma(z)$ is the Laplace transform of the friction memory kernel $\gamma(t)$. In particular, for GLE, $\gamma(t)$ can be given by $\gamma(t)=\frac{1}{m}\int_0^\infty\mathrm{d}\omega\frac{J(\omega)}{\omega}\cos(\omega t)$.

As usual, the average position and variance can be given by the Laplace transform and the residue theorem if the spectra of the noise is continuous [23] [24]. However, in order to form the current Debye spectra in this paper. $\hat{\gamma}(z)$ can be given as $\hat{\gamma}(z)\sim\arctan(z)$ [25]. In order to get ϕ_δ, the residue theorem needs to be used. The roots of equation $\left[z^2+z\hat{\gamma}(z)-\omega_b^2\right]^{-1}=0$ have to be known. Nevertheless, the equation has an infinite number of roots because special function $\arctan(z)$ is a multi-valued function. Thus the analytical result for the passing probability can not be given in a closed form [26]. For the sake of the effects of the absence of high frequency on the passing probability, numerical simulation is necessary and of great importance.

In order to study the thermally activated escape of a particle over a potential barrier, average position and variance of the particle must be obtained from above discussion. In the previous section, we have shown that the behaviour of dynamic variables in such a Debye spectrum is oscillation. Do these two variables of the particle still oscillate when crossing the potential barrier? How does the phenomenon of passing probability evolved over time? In **Figure 5**, we

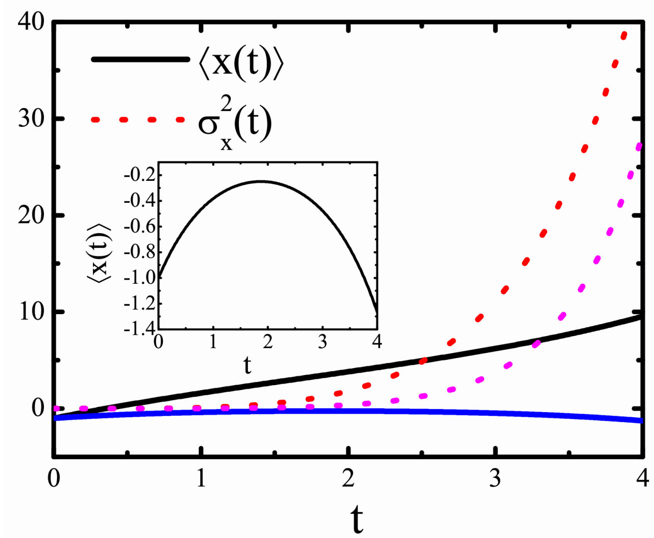

Figure 5. The average trajectory (solid lines) and variance (dotted lines) as function of time for initial velocity $v_0 = 3.0, 1.0$ from top to bottom (black solid line: $v_0 = 3.0$; blue solid line: $v_0 = 1.0$; red dotted line: $v_0 = 3.0$; purple dotted line: $v_0 = 1.0$). The average trajectory for smaller initial velocity is plotted in the inset. The parameters used are $T = 0.5$, $\omega_s = 0.5$, $x_0 = -1$, $\omega_b = 1.0$ and $\delta = 0.5$.

plot the time-dependent average trajectory and variance for different initial velocities. From this figure, an intriguing phenomenon can be observed that the dynamic variables $\langle x(t) \rangle$ and $\sigma_x^2(t)$ do not oscillate with time. Nevertheless, in the case of the inverse mechanism, the system is not equilibrated, at least with respect to a collective degree of freedom such as the reaction coordinate. The change of dynamic variables with time is not the oscillation. This behavior appears because the interaction of the particle with the external potential field occurs very quickly and the reaction time of the particle passing process is too short to observe the oscillation of dynamic variables with time. This implies that for the environment of the absence of the high frequency, e.g. Debye spectrum, the passing probability approaches a constant in the large time limit. This also provides a favorable basis for further research on how the truncation of high frequency affects the passing probability.

In **Figure 6**, we plot the passing probability of the sub-Ohmic particle as a function of high frequency cut ω_s with different initial energy. It is seen that the probability of passage varies nonmonotonically with the truncated frequency ω_s as the initial energy of the particle is small. For $\omega_s = 0$, *i.e.*, without thermal fluctuations. It is clear that particle will not be able to pass over the barrier if the initial particle energy is smaller than the height of the potential barrier. Once ω_s is increased to a small value, thermal fluctuations arise. As a consequence, the particle has more probability to overcome the potential barrier. Nevertheless, increasing the high frequency is not conducive to the particle crossing the barrier. It can be understood well by the friction of the system. In the case of larger high frequency cut. Namely, the vibration frequency of the environmental

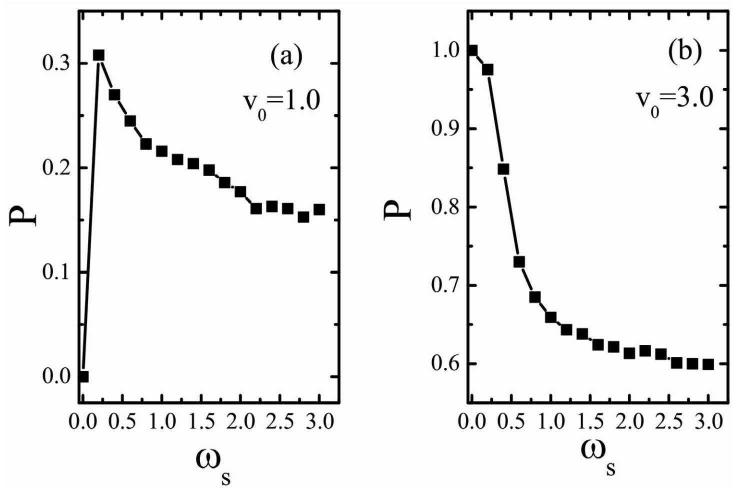

Figure 6. The passing probability as a function of ω_s for various initial velocity at fixed $\delta = 0.5$. The parameters used are $T = 0.5$, $\omega_b = 2.0$, and $x_0 = -1$.

oscillator is very high. The damping in such environment is going to be very large. The recovery of system instability will be faster. Because of the much energy consumption of the particle before crossing the barrier, the passing probability is reduced. It is worth pointing out that this nonmonotonic phenomenon can only occur when the initial energy is less than the barrier height. Obviously, the probability of passage decreases monotonically with truncated frequency if the initial energy is larger than barrier height.

4. Summary

Considering the truncation property of the generalized Debye spectrum, nonequilibrium characteristics of the system and the dynamics of the particle have been investigated in this paper. The oscillation behavior of the velocity autocorrelation function with time in a free field is analyzed. Remarkably, this oscillation is related to the speed of particle diffusion. Slower diffusion of the particle is favorable to the nonequilibrium observation of the system. In order to analyze further the equilibrium characteristic behavior subjected by such finite noise spectrum, we put the particle in an external potential, for instance a harmonic potential, respectively. For the case of a harmonic potential, we show that the system will not equilibrate when the noise spectrum is of the form of a Debye spectrum. As we expected, we find that making the system nonlinear restores thermal equilibration. Besides, the nonergodicity of the second kind of a harmonic particle subjected to an internal colored noise with generalized Debye spectrum is investigated. Moreover, by using numerical simulation techniques, the stable passing probability turns out to be a nonmonotonic function of the Debye phonon frequency. This phenomenon can be only observed when the initial energy is less than the barrier height. It is due to the fact that the larger lack of high frequency, the smaller the corresponding damping. Thus, the particle can easily to overcome the barrier and run to the other side of the potential.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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