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Frequency-dependent conductivity of Brownian particles in bistable and metastable structures

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The authors aimed to investigate the dynamic proprieties of one-dimensional system of Brownian particle immersed in bistable and metastable periodic potential, in other words in periodic potentials with two wells. The calculations are developed by using the Fokker-Planck equation which is solved numerically by the continued fraction expansion method (CFEM), in order to calculate the frequency-dependent conductivity. Our numerical results are given for various forms of the periodic potential and for different temperatures *T*. As expected, we found that the dynamical properties are very sensitive to the structure of the periodic potential. Moreover, our calculations show that the diffusive regime of particles in bistable periodic is slightly more important than the one calculated in metastable or in cosine forms. All calculations presented here are performed in the overdamped regime.

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1. Introduction

The one-dimensionnal diffusion of a Brownian particles in periodic medium represents a model that can be applied in numerous contexts, for it has possible applications in condensed matter physics, chemical-physics and molecular biology [1-4]. In the simplest Langevin equation, the particle is coupled to the environment by the viscous damping coefficient γ (which models the energy exchange with the substrate) and by a white noise, which are related to each other by the fluctuation-dissipation theorem [5]. These descriptions do not introduce an artificial distinction between local motion (oscillations) and diffusive motion. They thus allow a unified description of both essential dynamical features of the motion of the mobile particles. The determination of the dynamic properties of the system for arbitrary temperature and periodic potential remained a challenging task for decades, even at the over-damped limit. In the specifically case of a cosine potential, which is an oversimplification, the problem has been studied mainly from the point of view of the calculation of diffusion coefficient *D* and of some correlation functions, such as the velocity-velocity correlation spectrum, and the mean-square displacement [6,7]. These investigations are well understood, but there is only limited information for dynamic properties in effective potentials. However, in order to describe various systems in condensed matter physics and biology, more complicated potentials than the simple sawtooth type potential may be required. The present contribution continues our study [8,9] of Brownian motion in periodic potentials, considering the case when there are two potential barriers per period such as metastable and bistable potentials. The role of these potentials in the diffusion motion was pointed out in Refs [10,11] in the context of superionic conductors. The molecular-dynamics simulation of self-diffusion on metal surfaces [12] and experimental data for superionic conductors [13] provide the evidence that the potential barriers of different heights are important for the understanding of transport processes in corresponding systems. As mentioned in the beginning, our calculations are performed in the case of one dimensional system by solving the Fokker Planck equation using the continued fraction expansion method. The attention will be focused on the frequency-dependent conductivity, which provides important information about dynamic properties of diffusion process. Indeed, by varying the ratio $\xi = V_2/V_1$ (where V_2 and V_1 are the barriers of the potential) strictly between 0 and 1, we demonstrate the influence of the periodic potential structures on the behavior of Brownian particles in metastable and bistable potential. It is worthwhile to point out that the information on the dynamic phenomena is very useful for the applications

The present paper is organized as follows. In the second section the model is defined and the basic Fokker-Planck equation is set up. This equation is solved using the continued fraction expansion method. Numerical solutions for the frequency dependent conductivity are presented in the third section. Results can be obtained for large friction constants as well as for different periodic potential shapes. The concluding results will be given in the last section.

2. Theoretical model and method of calculation

The physical quantity which characterizes the dynamics of the diffusing particles can be expressed in terms of correlation functions. As mentioned in the introduction we will be interested to the frequency-dependent conductivity $\sigma(\omega)$ which is given by the Fourier transform of the velocity-velocity correlation function

$$\sigma(\omega)=\frac{\mathrm{Q}^2}{k_B TL}\int \mathrm{e}^{\mathrm{i}\omega t}\langle v(t)v(0)\rangle. \tag{1}$$

Where L is the chain length and Q is the particle's charge of system. The low frequency limit of the quantity $\sigma(\omega)$ is proportional to the diffusion coefficient D:

$$D=const\times\lim_{\omega\to 0}\sigma(\omega). \tag{2}$$

The correlation function can be calculated with the help of the transition probability density $f(x',v',t/x,v)$ in the phase space (x,v) of all mobile particles. This function determines the probability that a particle initially prepared at positions x' and velocity v' will be found at x and v after time t. It is determined by the Fokker-Plank equation (FPE):

$$\frac{\partial f(x',v',t/x,v)}{\partial t}=L_{FP}f(x',v',t/x,v). \tag{3}$$

With the Fokker –Planck operator expressed as:

$$L_{PF}=-v'\frac{\partial}{\partial x'}-\frac{k(x')}{m}\frac{\partial}{\partial v'}+\gamma\left(1+v'\frac{\partial}{\partial v'}+\frac{k_B T}{m}\frac{\partial^2}{\partial v'^2}\right). \tag{4}$$

Where m, γ and T are the masse, the friction coefficient and the temperature of the thermal bath, respectively. The quantity $k(x)=-\dfrac{\partial V}{\partial x}$ is the force acting on the particle derived from the potential $V(x)$, which is of a particular interest in this work. We shall come back to this potential in some of our considerations in section III.

Several methods for solving Fokker-Plank equation have been used, such as simulation method and eigen-function expansion [1]. In this work we use the continued fraction expansion method (CFEM) introduced by Zwanzing and Mori to solve such evolution equation [14]. The dynamical conductivity can be formally represented by a continued fraction [15]:

$$\sigma(\omega)=\frac{\beta Q^2}{L}\cfrac{a_0}{-i\omega+b_1+\cfrac{a_1}{-i\omega+b_2+\cfrac{a_2}{-i\omega+b_3+\ddots+\cfrac{a_{p-1}}{-i\omega+R_p(\omega)}}}} \tag{5}$$

where $\beta=\dfrac{1}{k_B T}$ and a_p , b_p are static correlation functions. The remainder $R_{p(\omega)}$ is a memory function which must be calculated approximately.

According to the algorithm technique developed by Zwanzig-Mori [12], the first few coefficients of the conductivity are given by:

$$a_0=\frac{k_B T}{m}. \tag{6}$$

$$a_1=\left(-\frac{1}{mk_B T}\right)\langle k(x)^2\rangle_0. \tag{7}$$

$$a_2=\frac{1}{m^2 a_1}\left[\langle k'(x)^2\rangle-\langle k'(x)\rangle^2\right]. \tag{8}$$

Where $k'(x)$ is the derivative of the force $k(x)$. The coefficients b_p are damping terms, which vanish in the Hamiltonian case $(\gamma=0)$

$$b_1=\gamma \;\; ; \;\; b_2=0 \;\; ; \;\; b_3=\gamma \;\; ; \ldots. \tag{9}$$

In order to calculate the dynamical conductivity by applying CFEM, one has to answer two principal questions. The first consists of finding a suitable approximation of the remainder of the infinite continued fraction. In the large friction limit, it is obtained by $R_p=\gamma$. The second problem appears in the evaluation of the static correlation functions.

3. Results and discussion

Considering a form of the potential $V(x)$ by taking the first two terms of the Fourier expansion of the periodic potential, then we can write

$$V(x) = A\cos(q_0 x) + B\cos(2q_0 x). \qquad (10)$$

As mentioned above, our study was performed by using the potential given in Eq. (10) for various values of ξ which is defined as the ratio of the two different barriers of the potential. The choice of the parameters A and B determine the desired values of the ration ξ and the shape of the periodic accorded to their sign. In fact, the bistable potential can be obtained when both constants A and B are positives while the metastable potential when they are negatives. Figs. 1 and 2 depict the shape of this potential in the case of bistable and metastable structure, respectively. We note that for varying the parameter ξ = V_2/V_1, we vary only the height of the barrier V_2 inside de cell , the other barrier V_1 outside the cell is chosen to be constant and equal to 0.1eV (see Figs. 1 and 2).

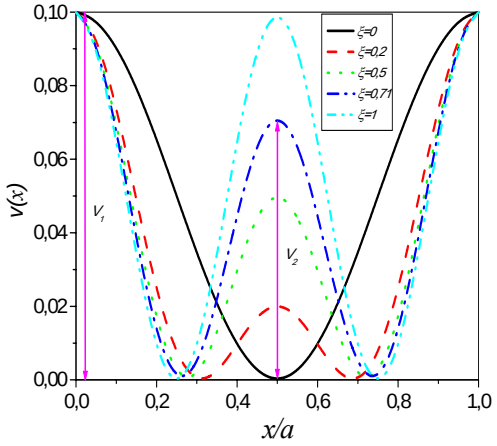

Fig. 1. Structure of the symmetric bistable potential V(x) for different values of the ratio of two potential barriers ξ.

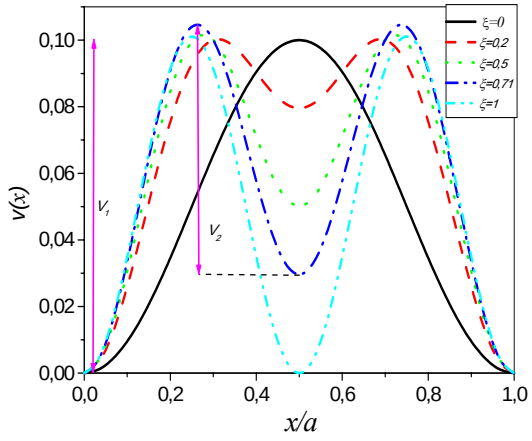

Fig. 2. Structure of the symmetric metastable potential V(x) for different values of the parameter ξ.

As mentioned above, the continued fraction method expansion is a powerful method to study dynamic properties for wide range of parameters of system. The principal problems arise only at extremely low friction. In this limit, the computational efforts are different: higher order continued fractions are necessary and no analytical solutions are then available. But, in many cases, at high temperatures or in high and intermediate friction regimes a few poles are sufficient to describe qualitatively the dynamic proprieties. In our case, a continued fraction expansion up to order 3 is used:

$$\sigma(\omega) = \frac{\beta Q^2}{L}\cfrac{a_0}{-i\omega + b_1 + \cfrac{a_1}{-i\omega + b_2 + \cfrac{a_2}{-i\omega + R_3(\omega)}}}. \qquad (11)$$

Within our model potential given by Eq.(10), the static correlation functions which soon become very lengthy are expressed as:

$$a_1 = \frac{q_0^2}{Nmk_B T}\left(A^2\left\langle \sin^2(q_0 x)\right\rangle_0 + 4B^2\left\langle \sin^2(2q_0 x)\right\rangle_0 + 4AB\left\langle \sin(q_0 x)\sin(2q_0 x)\right\rangle_0\right) \qquad (12)$$

$$a_2 = \frac{q_0^2}{Nm^2 a_1}\left(A^2\left\langle \cos^2(q_0 x)\right\rangle_0 + 16B^2\left\langle \cos^2(2q_0 x)\right\rangle_0 + 8AB\left\langle \cos(q_0 x)\cos(2q_0 x)\right\rangle_0 - \left\langle A\cos(q_0 x) + 4B\cos(2q_0 x)\right\rangle_0^2\right) \qquad (13)$$

The ensemble averaging (<…>) is calculated from the equilibrium distribution of Boltzmann by use the continued fraction expansion method. Then, we can easily calculate the dynamic conductivity $\sigma(\omega)$ as function of oscillation frequency ω.

A. Bistable model

In the following, we present and discuss qualitatively the motion of particles in the regime of large friction, i.e., for $\Gamma = \dfrac{2\pi\gamma}{\omega_0} >> 1$, where $\omega_0 = \left(\dfrac{2\pi}{a}\right)\sqrt{\dfrac{V_1}{2m}}$ is the characteristic frequency for vibration at the bottom of the well when the parameter ξ goes to zero (ξ=0).

Fig. 3 shows the variation of dynamic conductivity as a function of the frequency for different values of ξ in the limit of high friction limit. For extreme values of ξ (ξ=0, ξ=1) the specter of $\sigma(\omega)$ dominated by an oscillator peak situated at frequency around ω_0 and $2\omega_0$, respectively. In this situation, the particle spends the most part of the time by making small-amplitudes oscillations around the well bottoms, and sometimes is activated and makes a jump from a well to another.

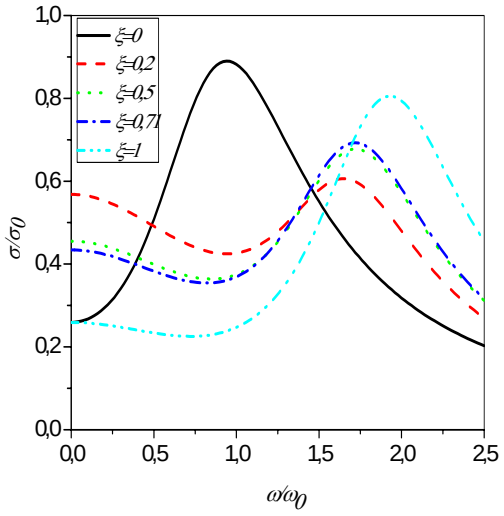

Fig. 3. Dependence of dynamic conductivity $\sigma(\omega)$ *with the frequency* ω *for different values of* ξ*. The other parameters are* $\Gamma=7$*,* $T=300$ *K,* $V_1=0.1eV$*.*

For the other values of ξ, the behavior of the conductivity $\sigma(\omega)$ behaves differently, as is visible from the figure. Indeed, when the parameter ξ decreases the oscillatory peak decreases and the central peak ($\omega=0$) increases strongly in intensity. This finding, suggests then that for low values of ξ, the particle motion is mainly of diffusive motion.

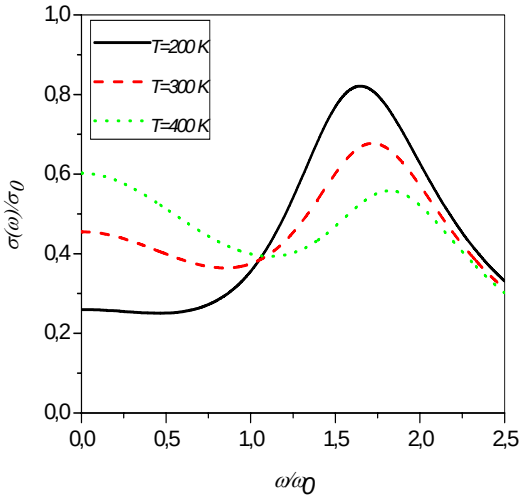

Fig. 4. Dependence of dynamic conductivity $\sigma(\omega)$ *with the frequency* ω *for different values of* T *the other parameters are* $\Gamma=7$ *and* $\xi=0.5$*.*

This transition from the oscillatory to the diffusive regime in our model potential can be also achieved, as the temperature increases (see Fig. 4). In fact, for a fixed value of ξ (ξ =0.5 for example) and at T=200 K, a strong oscillatory peak appears approximately at the frequency $\omega=1.7\omega_0$. At intermediate temperature T=300 K, this peak moves slightly to lower frequencies and decreases in intensity. At T=400 K, the central peak increases and the oscillatory continues to decrease in intensity, reflecting the important diffusive motion of the particles over the potential barriers. Furthermore, if the temperature is high compared to the barrier height ($k_BT >> V_1$), the dynamic response of the Brownian particle becomes that of a freely diffusing particle.

B. Metastable model

In this subsection, as for the previous one, we illustrate the behavior of the dynamic conductivity of our Brownian particles immersed in metastable potential in the limit of high friction. The results for $\sigma(\omega)$ obtained from the continued fraction expansion method are shown in Fig. 5, for different values of ξ.

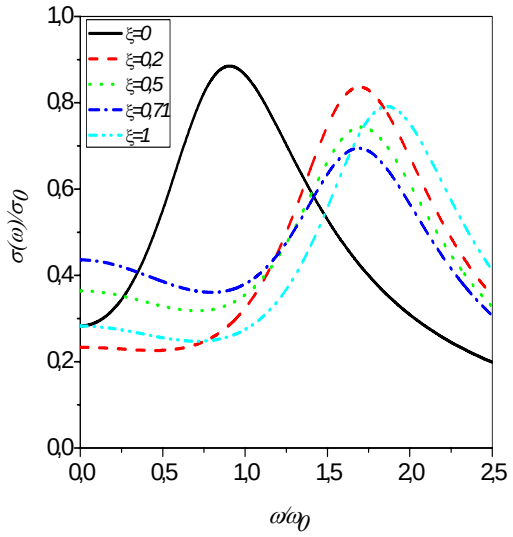

Fig. 5. Dependence of dynamic conductivity $\sigma(\omega)$ *with the frequency* ω *for different values of* ξ*. The other parameters are* $\Gamma=7$*,* $T=300$ *K,* $V_1=0.1eV$*.*

As expected, for the extreme values of ξ, we obtain the same behavior of the conductivity as for bistable potential. Because, for these two values of ξ, both structures (bistable and metastable) coincide, justifying then the same spectrum obtained for the conductivity. For the other values of ξ, we observe that contrary to bistable potential, the increasing of the ξ has the effect of increasing slightly the central peak. On the other hand, the spectrum of the conductivity remains dominated by the oscillatory peak, reflecting the importance of the oscillatory regime in metastable structure.

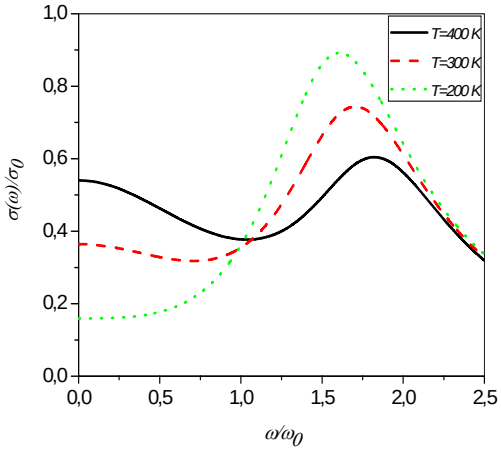

Fig. 6. Dependence of dynamic conductivity $\sigma(\omega)$ with the frequency ω for different values of T. The other parameters are Γ=7, ξ=0.5 and, V_1 =0.1eV.

However, the transition from the oscillatory to the diffusive regime is clearly seen, as the temperature increases (see Fig. 6).

Finally, in order to make a quantitative comparison we have plotted in one figure as is seen in Fig. 7 the conductivity versus the frequency for the three forms of periodic potential: bistable, metastable and cosine potential. The analytical expression of cosine potential used here, is given by:

$$V(\mathrm{x}) = \frac{V_1}{2}(1-\cos(q_o x)). \qquad (14)$$

The analysis of this figure shows that the conductivity at zero frequency is more important for bistable potential than the one calculated for metastable and for a usual cosine potentials. Whereas for high frequency, the situation is different and opposite: the big intensity of the oscillatory peak is found for cosine potential and the low intensity is found for the bistable potential.

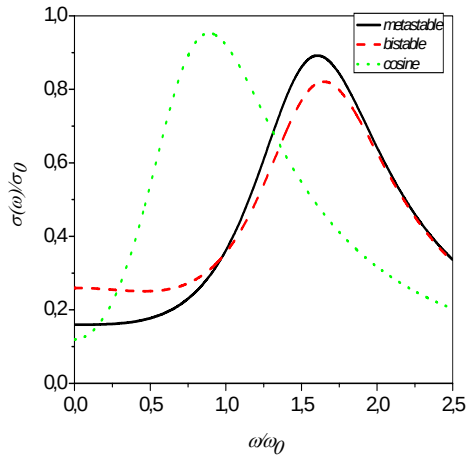

Fig. 7. Dependence of dynamic conductivity $\sigma(\omega)$ with the frequency ω for the three forms of periodic potential the parameters are Γ=7, T=200 K and ξ=0.5.

4. Conclusions

The intention of this work was to study the dynamic proprieties of one-dimensional system of Brownian particles subject to symmetric bistable and metastable potential, being obviously more realistic and flexible for possible applications in condensed matter physics and biology.

While such systems have been of interest for several decades, our interest is motivated by the fact that, we have not found much work in the literature on dynamic proprieties in these potential shapes. For this purpose, we have focused our attention mainly on the frequency-dependent conductivity $\sigma(\omega)$. The calculations of $\sigma(\omega)$ are developed for a wide range of frequency by using the Fokker-Planck equation which is solved numerically by the continued fraction expansion method (CFEM) truncated at the four order. By varying the ratio of the barriers $\xi = V_2/V_1$ strictly between 0 and 1, we demonstrate the influence of the periodic potential structures on the behavior of Brownian particles in metastable and bistable potential. Our calculations show that the diffusion regime in bistable periodic potential is slightly more important than the one calculated in metastable or in cosine form.

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