Fokker-plank dynamic in a general periodic potential shape

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A general theory for diffusion mechanism of Brownian particle submitted to a bistable and metastable periodic potential is presented. It is based on the description of the kinetics in the framework of Fokker-Planck equation (F.P.E). A formal solution of the F.P.E is obtained using the Matrix Continued Fraction Method (M.C.F.M), which gives an expression for the relevant correlation function. In particular, the half width of the quasi-elastic peak of the dynamical structure factor *S(q,)* and the diffusion coefficient are fully studied in a wide range of physical parameters. A comparison between the results of system in a bistable and those in a metastable potential is presented and analysed.

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I. INTRODUCTION

The understanding of diffusion particle is of central importance in many process such as superionic conductors (S.I.C) [1]. These materials can generally be thought of as consisting of two structural sublattices, a rigid immobile structural through which the conducting species is more or less free to move, and the mobile ions themselves. These solids with high ionic conductivity are of great current interest due both to their technological importance and the physics involved in their behaviour[2]. Some of the essential dynamical properties of S.I.C have successfully been described by one particle model which treats the mobile cations as Brownian particles [3] subject to a periodic potential [4,5] provided by the anion lattice. Our main purpose in the present paper is to illustrate the effect of the ratio of the two barriers of metastable and bistable periodic
potential on the diffusion process. Starting from the FPE and using the matrix continued fraction method, we have calculated the half width at half maximum(HWHM) $\lambda(q)$ of the quasi-elastic line of $S(q,\omega)$ up to large values of q for different shape of potentials and for different temperature regimes. For different ratios of potential barriers Δ ($\Delta=V_2/V_1$) and for different friction regimes, the diffusion coefficient is obtained by an analysis of the energy width of the dynamic structure factor.

II. POTENTIAL MODEL

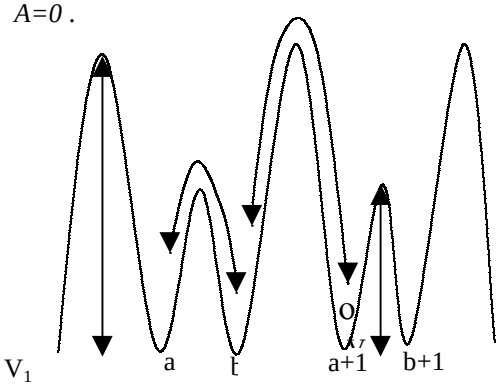
From the point of view of the classical theory of stochastic processes the diffusive motion of a Brownian particle of mass m with friction constant γ is described by the Fokker-Planck equation:

$$\frac{\partial W}{\partial t} = -v\frac{\partial W}{\partial x} + \frac{1}{m}\frac{\partial V(x)}{\partial x}\frac{\partial W}{\partial v} + \gamma\frac{\partial}{\partial v}(v + \frac{k_B T}{m}\frac{\partial}{\partial v})W \quad (1)$$

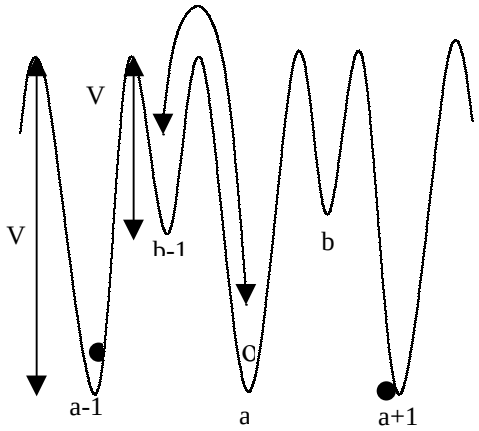
where $W(x,v,t)dx\,dv$ is the probability of finding the particle in the phase space element between (x,v) and $(x+dx, v+dv)$. $V(x)$ is the periodic potential which we choose in the following form[6]:

$$V(x) = A\cos(q_o x) + B\cos(2q_o x) \quad (2)$$

with two barriers $V_1(A, B, q_o)$ and $V_2(A, B, q_o)$. $q_o=2\pi/a$ where a is the lattice constant. Our investigations were performed using the potential given by Eq.(2) for various values of Δ ($\Delta=V_2/V_1$) and for two different shapes of periodic potential (see schema 1 and schema 2), noting that $\Delta=0$ corresponds to $B=0$ and $\Delta=1$ corresponds to $A=0$.



Schema 1



Schema 2

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When a particle moves in this type of periodic potential, two different diffusion mechanisms are possible, depending on the first barrier height V_2 compared to the thermal energy k_BT. For the low value of barrier V_2, the particle makes small-amplitude oscillations around the well bottoms and makes a jump from a well to another, by overcoming the second barrier height V_1. If the barrier V_2 is sufficiently high, the particle makes a jump from a well to another (a---b) and jump from b to a+1. In a previous paper[7], we have shown that for strongly interacting Brownian particles in two-dimensional periodic potential, the effective potential computed along the direction where the system is incommensurate presents the same shape as the one chosen in the first case of this section. In the second one, by inverting the symmetric bistable potential we get the metastable potential, which we present in schema 2. In this form of potential, we notice two types of sites a and b.
Once the particle has escaped an a-type well, it may be retrapped in a nearest-neighbour one (b-type) or it may make a flight after which is captured in an another a-type. A particle jumps rapidly from a b-type to an unoccupied a-type well, but the jump from a-type to b-type well is much slower.

Exact numerical results for diffusion in such types of potential (schemas 1 and 2) can be obtained by solving the Fokker-Planck equation in position and velocity variables by the Matrix continued fraction method (MCFM)[8,9]. In this way, the Green function of the FPE and the dynamical structure factor $S(q,\omega)$ can be obtained. From $S(q,\omega)$, the diffusion coefficient D may be computed via the Kubo relation [10].

III. MATRIX CONTINUED FRACTION METHOD

A. DYNAMICAL STRUCTURE FACTOR

As mentioned elsewhere, a reliable numerical method for calculating the diffusion constant is based on the half-width of the quasi-elastic peak of the dynamic structure factor $S(q,\omega)$ [11,12]. The studies performed by means of FPE in periodic potential showed that, at fixed q, $S(q,\omega)$ presents a quasi-elastic peak, centered around $\omega=0$, which properly describes the diffusive motion of the particle. At very high friction γ, $S(q,\omega)$ is a monotonously decreasing function of ω, but with the low value of friction and at high barriers, the dynamical structure factor $S(q,\omega)$ presents secondary peaks connected to the oscillating dynamics around the minimum of potential [13], the dynamical structure factor can be calculated via a MCFM [14,15] and $S(q,\omega)$ is the time Fourier transform of the characteristic function $F(q,t)$. In the following, we give only the essential lines of the method. The details can be found in Ref [14,15]

$$S(q,\omega)=\frac{1}{2\pi}\int e^{i\omega t}F(q,t)dt \tag{3}$$

with

$$F(q,t)=\langle e^{-iq(x-x_0)}\rangle \tag{4}$$

The brackets < ... > represent statistical average and x and x_0 refer to the same diffusing particle.

The dynamical structure factor can then be written, in the first Brillouin zone as:

$$S(q,\omega)=NRe\left\{\sum_{p,r=-\infty}^{\infty}\tilde{G}_{0,0}^{p,r}(k,i\omega)M_{p-l}M_{r-l}^{*}\right\} \tag{5}$$

where

$$M_r=\frac{1}{2\pi}\int_{-\pi}^{\pi}\exp(-\frac{V(x)}{2}+irx)dx$$

the integrals M_r are completely defined by the potential $V(x)$. $\tilde{G}_{0,0}(k,i\omega)$ is expressed by matrix continued fraction:

$$\tilde{G}_{0,0}(k,i\omega)=\cfrac{I}{i\frac{a}{2\pi}\sqrt{\frac{m}{k_BT}}\omega I+B^{+}\cfrac{I}{\frac{a}{2\pi}\sqrt{\frac{m}{k_BT}}(i\omega+\gamma)I+2B^{+}\cfrac{I}{\frac{a}{2\pi}\sqrt{\frac{m}{k_BT}}(i\omega+2\gamma)I+\ldots}B^{-}}B^{-}} \tag{6}$$

In equation (6) I is the identity matrix and the matrice elements B^{+} and B^{-} are given by the following equations:

$$B^{+}_{p,r}(k)=(p+k)\delta_{p,r}+\frac{A}{4k_BT}(\delta_{p,r-1}-\delta_{p,r+1})+\frac{B}{2k_BT}(\delta_{p,r-2}-\delta_{p,r+2})$$
$$B^{-}_{p,r}(k)=(p+k)\delta_{p,r}-\frac{A}{4k_BT}(\delta_{p,r-1}-\delta_{p,r+1})-\frac{B}{2k_BT}(\delta_{p,r-2}-\delta_{p,r+2}) \tag{7}$$

We first notice that, for practical purposes, the infinite summation in Eq.(5) must be truncated.

The dimension of the matrices employed and the number of iterations in the continued fraction must be chosen in order to ensure a good convergence of the results. The speed of convergence depends also on the value of friction. The MCFM becomes very cumbersome at low friction, while it is more precise and convenient at high friction.

Let us analyze the behavior of the HWHM $\lambda(q)$ in two cases of potential (bistable and metastable potential) and for different values of the ratio of two potential barriers Δ.

However for low values of Δ $(0<\Delta \leq 1/2)$, the shape of $\lambda(q)$ in the case of bistable potential differs completely from that in the metastable potential (see Figs.1 and 2). In fact, in the former case, we notice that for some values of Δ the pointed peaks which move toward the left appear. These peaks reflect the existence of liquid-like motion. While in the second case, the function $\lambda(q)$ is a periodic function of q. The mechanism of diffusion is described by jump process with jump length close to the lattice constant a. This indicates that the diffusion process in both types of potentials consists of a superposition of both liquid-like and hopping motion.

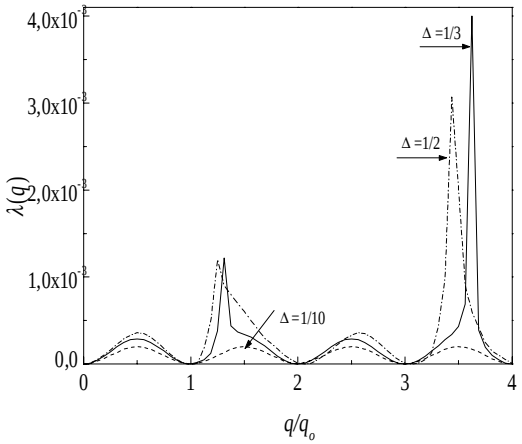

FIG1: Half width of the quasi-elastic line of $S(q, \omega)$ as a function of wave vector, for different low values of Δ (Δ is the ratio of barriers bistable potential) in case of potential bistable at low temperature $K_BT=V_1/6$ and high friction $\Gamma=36$.

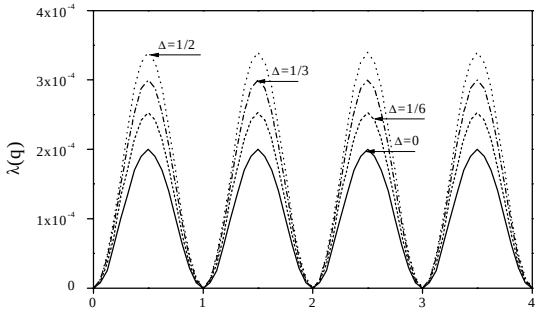

FIG 2: Half width of the quasielastic line of $S(q, \omega)$ as a function of wave vector, for different low value of Δ (Δ is the ratio of barriers metastable potential) in case of metastable potential at low temperature $K_BT=V_1/6$ and high friction $\Gamma=36$.

B. DIFFUSION COEFFICIENT

The aim of this section is to describe diffusion process of a Brownian particle moving in both symmetric bistable and metastable. For that, we are interested in particular in the diffusion coefficient D which is an important quantity, since it can describe the intrinsic properties of the system. We are able to calculate the diffusion coefficient in two different limits : the high friction regime and the underdamped regime, characterized by energy diffusion. A true study of diffusion in all damping regimes can be performed essentially only by numerical methods developed in section (III). So, the diffusion coefficient D is obtained as:

$$D = \frac{a}{4\pi}\sqrt{\frac{m}{k_B T}}\lim_{q\to 0}\frac{\lambda(q)}{q^2} \qquad (8)$$

a is the lattice constant and $\lambda(q)$ is the half width of the quasi-elastic peak of $S(q,\omega)$. The equation (8) means that the small q behaviour of $\lambda(q)$,which is usually investigated in neutron and atom scattering experiments, gives the diffusion coefficient.

We apply these formulas which were presented in the last paper [11] to calculate the diffusion coefficient D in both bistable and metastable periodic potential for different values of friction $\Gamma = 2\pi\gamma/\omega_0$,where $\omega_0 = (2\pi/a)(V_1/2m)^{1/2}$ is the characteristic frequency for vibration at the bottom of the well when Δ =0.

Let us now make a comparison between the diffusion process in bistable and metastable periodic potential, for two extreme limits of friction i.e. at high and low friction. In Fig. 3, we notice that in the high friction limit the diffusion coefficient of system moving in a bistable potential coincide with that in a metastable potential. This agreement can be well explained in terms of vibration frequencies at the bottoms ω_b and the tops ω_s point of the potential $V(x)$. In fact, the product $\omega_b\omega_s$ has the same value in both bistable and metastable periodic potential for every value of Δ. This is due essentially to the fact that we can get the metastable potential only by inversion of the bistable potential and vice-versa. We recall that, in this regime of friction, the jump probability $\phi\left(\phi = D/a^2\right)$ is approximately defined by [16] : $\phi \propto \frac{\omega_b\omega_s}{2\pi\gamma}$

In the low friction regime, (Fig.4) we notice that the behaviour of D in bistable potential is different from the one in metastable potential, particularly in the low value of Δ . as above, this discrepancy can be understood from the dependence of the vibration frequency in the deepest well ω_b , with Δ. In effect, in the low friction regime the jump probability ϕ is proportional to ω_b($D \propto \omega_b$). Hence by increasing slightly the value of Δ the vibration frequency at the bottom increases in the case of metastable potential and decreases for the bistable potential.

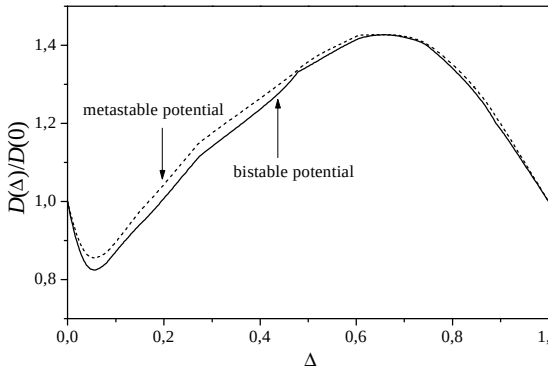

FIG 3: Diffusion coefficient *D* of system in both bistable and metastable periodic potential, as a function of *Δ*.The parameters are $V_1=0.1eV$, $K_BT=V_1/6$ *and* $\Gamma=36$

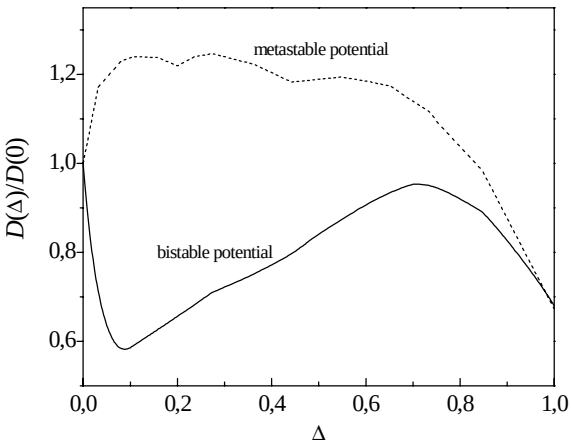

Fig 4 : Same as Fig 3 but for low friction Γ =1.5

IV. CONCLUSION

In this paper, we have studied the diffusion process of particles moving in both symmetric bistable and metastable potentials described by the Fokker-Planck equation. The method used for solving this equation is the matrix continued fraction method. We are particularly interested in the half-width at half maximum $\lambda(q)$ of the dynamical structure factor $S(q, \omega)$ and the diffusion coefficient. The behaviour of $\lambda(q)$ shows that the diffusion process in symmetric bistable potential, can be described by a superposition of both hopping and liquid-like motion. Whereas in case of symmetric metastable potential, the behaviour of the system can be described by the hopping motion with different probabilities of jump[17]. The important result here, is that the diffusion is highly sensitive to the structure of the periodic potential only in the low friction regime.

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