Fokker Planck Dynamic in a Periodic Triple-Well Potential

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In this work we present a general theory for diffusion mechanism of Brownian particle submitted to a symmetric and periodic triple-well potential (Fig 1). The kinetics description is done with a Fokker-Planck equation (F.P.E). The F.P.E is resolved numerically using the Matrix Continued Fraction Method (M.C.F.M).In order to calculate some important correlation functions. The half-with of the quasi-elastic line λ(q) of dynamic structure factor S (q,w) is studied in the high friction regime and low temperature for different structure of potential with a fixed barrier potential The result show that the half with λ(q) present the same aspect for different values of the ratio of two potential barriers Δ (Δ=V_1/V_2), except for Δ≈1 for which λ(q) is a cosine function.

PACS. 05.40.-a fluctuation phenomena, random processes, noise and Brownian motion-66.30.Dn Theory of diffusion and Ionic conduction in solids.

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I- INTRODUCTION:

The diffusion of Brownian particles in a periodic potential is one of the interesting problems which has been studied in many different scientific areas [1]. It represents a model that can be applied to numerous systems, ranging from superionic conductors and intercalation compounds to submonolayer films adsorbed on surfaces of crystalline substrates. The common features of these systems are that they consist of two species of particles; one species is fixed around certain equilibrium sites and forms a regular lattice while the other species is mobile and moves through this lattice. These systems are characterised by diffusion constants in the range of liquids, but the periodicity due to the crystalline substrate, is not completely lost. If the diffusing particle is sufficiently massive, the diffusion problem can be treated within a classical approach. The theoretical method to understand this important problem has been developed mainly in two directions. The first is numerical molecular dynamics or the Monte Carlo simulation method [2]. The second method is an analytical study based on the Langevin or the Fokker-Planck equation (also called a forward Kolmogorov equation) describing the Brownian potential [5, 6].The diffusion problem in symmetric and asymmetric double-well potentials has been recently investigated [7-11]. Here we shall be mainly concerned with the Fokker-Planck dynamics in a periodic triple well potential (Fig1), which is very interesting because it present intermediate wells that can accelerate the diffusion of particles [12, 13],

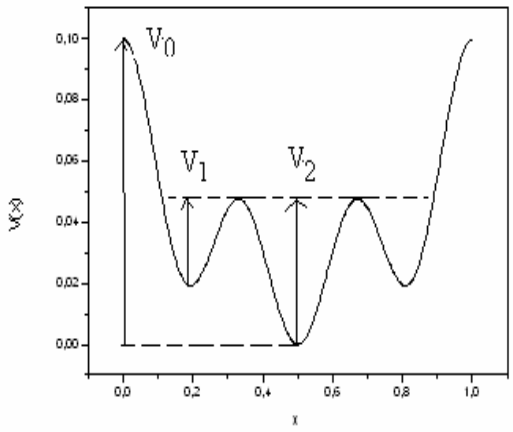

FIG. 1: The schema of symmetric triple-well potential.V_0=0.1eV.Δ=V_1/V

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II- MODEL AND METHOD: THE MATRIX-COUNTINUEDFRACTION METHOD (MCFM)

Both from a theoretical and an experimental point of view, the quantity carrying the most complete information on the correlations effects between the diffusing ions space and time is the coherent dynamic structure factor S (q, ω) defined (In 1D notation) as time Fourier transform of the characteristic function $F(q,t)$:

$$S(q,\omega)=\frac{1}{2\pi N}\int_{-\infty}^{+\infty} dt\exp(i\omega t)F(q,t), \quad (1)$$

With

$$F(q,t)=<\exp -iq(x(t)-x(0))> \quad (2)$$

where the angle brackets refer to the thermal average. x(t) and x(0) refer to the same particle. The derivatives of F (q, t) with respects to q, evaluated in q=0, gives the moments of the displacements distribution (even moments only differing from zero) and all the self-correlations functions can be deduced from S (q, ω), via the Green-Kubo relation [14] by doing suitable limits.

Let us illustrate how the average in equation (2) can be calculated. The starting point is the Fokker-Planck equation (FPE), which described the diffusive motion of a Brownian particle

$$\frac{\partial f(x,v,t)}{\partial t}=L_{FP}\,f(x,v,t) \quad (3)$$

With the Fokker-Planck operator L_{FP} :

$$L_{FP}=-v\frac{\partial}{\partial x}+\frac{1}{m}\frac{\partial V(x)}{\partial x}\frac{\partial}{\partial v}+\gamma\frac{\partial}{\partial v}\left(v+\frac{k_BT}{m}\frac{\partial}{\partial v}\right) \quad (4)$$

$f(x,y,t)\,dxdv$ is the probability of finding the particle to the phase space element between *(x,v)* and *(x+dx, v+dv)*, T is the temperature and k_B is the Boltzmann constant.

The Fokker-Planck equation cannot be solved analytically in every regime of frictions and potential barrier

The expression of the dynamic factor of structure is thus written in the following form

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

Where N is a normalized factor, q=2π/a(k+l) with $-\frac{1}{2}\prec k\le\frac{1}{2}$, l integer.

$$M_r=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp(-\frac{V(x)}{2}+irx)dx \quad (6)$$

M_r are some coefficients depending on the potential.

Defining the following quantity:

$$\xi=\frac{a}{2\pi}\sqrt{\frac{m}{k_BT}}$$

The Green function $G_{0,0}$ can be expressed as a continuous fraction of some matrices depending o the potential and the friction:

$$\tilde{G}_{0,0}(k,i\omega)=\cfrac{I}{i\xi\omega I+B\cfrac{I}{\xi(i\omega+\gamma)I+2B\cfrac{I}{\xi(i\omega+2\gamma)I+....}}\tilde{B}} \quad (7)$$

We will now apply the method described above in the case of a periodic potential tri stable, and the homogeneous friction. The V(x) potential is in the following form:

$$V(x)=A_1\cos(qx)+A_2\cos(2qx)+A_3\cos(3qx) \quad (8)$$

A_1, A_2 and A_3 determine the amplitudes of the three barriers of potential V_0, V_1 and V_2

In this case the matrices B and $\tilde{B}$ are given by the following equations:

$$B^{r,p}(k)=(r+k)\delta^{r,p}-\left[\frac{G_1}{2}(\delta^{r+1,p}-\delta^{r-1,p})+G_2(\delta^{r+2,p}-\delta^{r-2,p})+\frac{3}{2}G_3(\delta^{r+3,p}-\delta^{r-3,p})\right]$$

$$\tilde{B}^{r,p}(k)=(r+k)\delta^{r,p}+\left[\frac{G_1}{2}(\delta^{r+1,p}-\delta^{r-1,p})+G_2(\delta^{r+2,p}-\delta^{r-2,p})+\frac{3}{2}G_3(\delta^{r+3,p}-\delta^{r-3,p})\right]$$

$$G_1=\frac{q_0A_1}{2} \qquad G_2=q_0A_2 \quad G_3=q_0A_3$$

III- RESULTS AND DISCUSSIONS:

The result presented in Fig (2, 3) show that the half with λ(q) present the same aspect for different values of the ratio of two potential barriers Δ (Δ=V_1/V_2), except for Δ≈1 for which λ(q) is a cosine function with a period equal to three period of the potential. We remark that the intensity of λ(q) decrease whit Δ increase, that reflect the difficulty to jump over the barrier of potential that increase whit Δ. In the strong friction regime, the diffusion takes place by jump from one site to nearest neighbour one, independently of the structure of the potential, and the long jumps are cess likely [9,10]. So the curve represents the behaviour of the particle inside of the cell (of a site).The first pick (x=0.5) whit weak intensity represents the jump through V_0. The second

pick(x=1.5), big intensity represents the jump through V_1.Whereas the third pick (x=2.5) represents the jump through V_2.The presence of a middle well reduces the rate from left to right, relative to the double well case, so instead of crossing V_0, the particle crossed at first V_1 then V_2 to pass in a nearly close site. For $q/q_0>4$, one recovers the same behaviour of big intensity that reflects the motion of the particle inside of the cell near neighbour, but in the hydrodynamic limit.

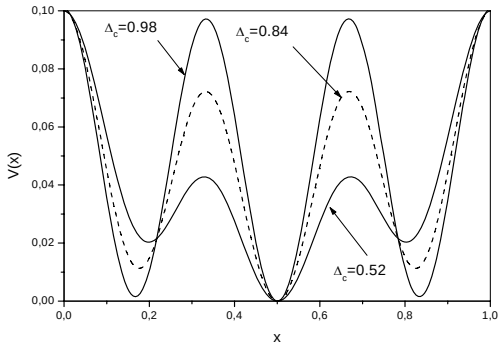

FIG. 2: Structure of the symetric triple-well potential$V^1(x)$ presented for different values of the ratio of two potential barriers Δ ($\Delta=V_1/V_2$).

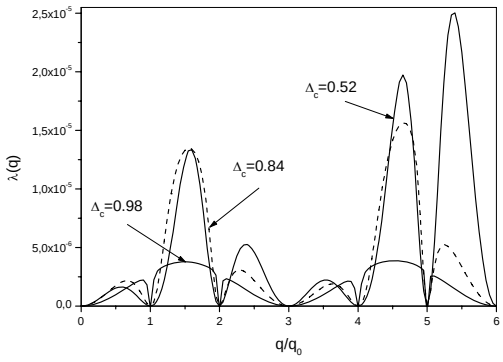

FIG. 3: The q-dependence of the half-with of the quasi-elastic line λ(q) of dynamic structure factor S (q,w) associated with different shapes of the tristable potential. The parametrs of this figure are V_0=0.1eV, $K_BT=V_0/6$ and Γ=10 (strong damping).

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