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Translocation time of periodically forced polymer chains

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In this work we study the presence of both a minimum and clear oscillations in the frequency dependence of the translocation time of a polymer described as a unidimensional Rouse chain driven by a spatially localized oscillating linear potential. The observed oscillations of the mean translocation time arise from the synchronization between the very mean translocation time and the period of the external force. We have checked the robustness of the frequency value for the minimum translocation time by changing the damping parameter, finding a very simple relationship between this frequency and the correspondent translocation time. The translocation time as a function of the polymer length has been also evaluated, finding a precise L^2 scaling. Furthermore, the role played by the thermal fluctuations described as a Gaussian uncorrelated noise has been also investigated, and the analogies with the resonant activation phenomenon are commented.

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I. INTRODUCTION

The transport features of molecules and polymers attract nowadays more and more interest. In particular, the translocation features of DNA polymers through pore cells have been studied with great attention [1] and different models have been introduced to describe such process. In between them we can mention for instance the single barrier potential [2] and the flashing ratchet models [3]. Despite all these efforts, the basic understanding of the translocation process of polymers is still missing. In many cases, the translocation phenomena involve also molecular motors [4,5] whose complex action has been only recently addressed with high attention. In addition, nanotechnological machines can learn from the biological processes and thus to work in a simpler and more efficient way [6]. The goal of this article is to study a cyclic time-dependent model that can depict a simple nanotechnological machine which is able to drive with a sinusoidal force a polymer chain in one direction. This simple object constitutes, in our purpose, a basic model that will be further developed into a more realistic machine able to emulate the basic behavior of a biological motor. We find a nontrivial behavior of the polymer translocation time as a function of the driving frequency ν with the occurrence of a series of oscillations. These oscillations are not related to the vibrational internal modes of the chain but to the driving frequency. The first minimum occurs at mean times $\tau_m \lesssim T_m$, where $T_m = 1/\nu_m$ is the period of the driving at this minimum. In this sense, the translocation time dependence presents some similarities with the resonant activation phenomena [7]. The polymer scaling properties have been checked and verified as a function of both the number of polymer beads, and the damping. The paper is structured in the following way: next section presents the model, then we report the results in Sec. III. In Sec. III C, the dependence of the stall force of the system is also studied, finding a strong nonmonotonic behavior with the frequency even in the presence of relatively high damping. We finish with a conclusions section.

II. MODEL

The polymer is modeled as a unidimensional chain of N dimensionless monomers connected by harmonic springs [8], whose total potential energy is

$$V_{\mathrm{har}} = \frac{k}{2}\sum_{i=1}^{N-1}(x_{i+1} - x_i - d_0)^2. \tag{1}$$

Here k is the chain elastic constant, x_i the position of the ith monomer and d_0 the equilibrium distance between adjacent monomers.

The translocation is helped by the presence of a linear potential (see Fig. 1) oscillating with frequency ν which acts in a space region of length L_M. In particular:

$$V_{\mathrm{sp}}(x,t) = \begin{cases} -F_0 x[1-\cos(2\pi\nu t + \phi)], & x \in [-L_M, 0] \\ 0, & \text{otherwise} \end{cases}. \tag{2}$$

The dynamics of the i^{th} monomer of the chain is then described by the following underdamped Langevin equation,

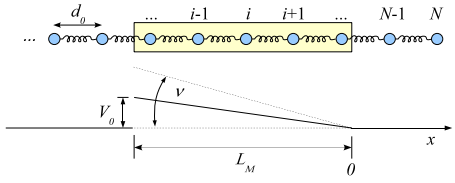

FIG. 1. (Color online) Scheme of the oscillating pushing force acting on a polymer chain formed by N monomers. The force drives only a small fraction of the whole chain.

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$$\ddot{x}_i + \gamma\dot{x}_i = -\frac{\partial V_{har}}{\partial x_i} - \frac{\partial V_{sp}}{\partial x_i} + \xi_i(t).$$

The polymer is subject to a viscosity parameter γ, being neglected other more complex hydrodynamical effects. Thermal fluctuations are described as Gaussian uncorrelated noise $\xi_i(t)$ which satisfies the usual statistical properties $\langle \xi_i(t)\rangle = 0$ and $\langle \xi_i(t)\xi_j(t+\tau)\rangle = 2\gamma D\delta_{ij}\delta(\tau)$ with $(i,j=1\ldots N)$. F_0 and ν represents, respectively, the amplitude and the frequency of the forcing field, and ϕ its initial phase.

The model here described represents a simple example of a driven polymer translocation, which may reveal as proper mechanism in nanotechnological devices and as a reference example in the area of the translocation driving machines. With this we mean a system which is able to push a polymer chain from one point to another, in analogy with a molecular motor which push a long molecule in the biological translocation process.

III. RESULTS

In this paper, we will focus on studying the dependence of the mean first passage time, as defined below, and of the stall force of the polymer with the frequency of the external driving. Simulations were done at different values of damping and noise (usually $\gamma = 1.0$ and $D = 0.01$) for $F_0 = 0.1$, $k = 1$, and $L_M = 5.5$. We have studied chains with $N = 12$, 18, 24, 36, and 120 monomers. The computed mean values are the result of averaging over 10^4 realizations. For each case we have integrated the Langevin equation of motion of the system by using a stochastic Runge-Kutta algorithm [15] with $dt = 0.01$, which is small enough for all the calculations here performed.

The initial spatial configuration of the polymer is put with all the beads lying at the rest distance $d_0 = 1$ with respect to each other, and the last sited at coordinate $x_N(0) = 0$, the final position of the external force region. Every simulation stops when the coordinate of the center of mass $x_{cm} = 1/N\Sigma_i^N x_i$ of the chain reaches the position $x_{cm} = 0$ and the mean first passage time (MFPT) is then computed as

$$MFPT = \tau = \frac{1}{2\pi}\int_0^{2\pi} \langle \tau(\phi)\rangle d\phi, \tag{3}$$

where $\tau(\phi)$ represent the FPT of a single realization, and ϕ is randomly chosen.

The adoption of the center of mass as reference point in the movement has the role of avoiding the boundary effects given by the spatial extension of the motor. In fact at the end of the translocation process of the full chain, the total force acting on the polymer is smaller because of the decreasing number of monomers inside the motor. The choice of the center of mass as a reference will preserve the calculations from this unwanted boundary effect, being the average number of monomers inside the motor always the highest possible. Figure 2 shows the MFPT τ as a function of the frequency of the oscillating force for damping parameter $\gamma = 1$, which corresponds to a quite damped condition for the system. A clear minimum is visible at a resonant frequency $\nu_m \sim 6\times 10^{-3}$. Moreover, a very strong oscillating behavior appears in the region $\nu \in [4\times 10^{-3} - 4\times 10^{-2}]$, before the high frequency saturation value is reached.

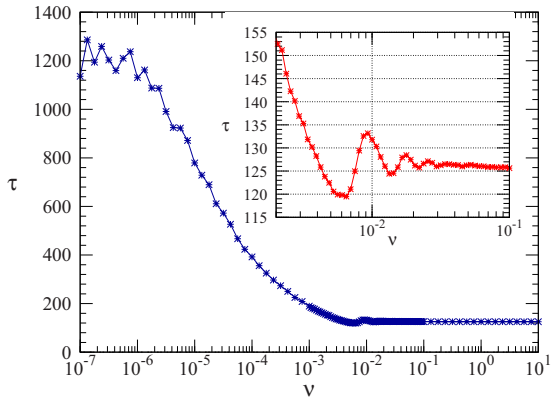

FIG. 2. (Color online) Log plot of the mean first passage time τ as a function of frequency of the oscillating force for the damping parameter $\gamma = 1$. The minimum and the oscillating behavior is showed in the inset. The thermal noise intensity is $D = 0.01$. The first minimum, which is also the global one, satisfies the very robust condition: $\nu_m^{-1} = T_m = \alpha\tau_m$, were α is a constant.

The thermal noise intensity is given by $D = 0.01$. Temperature acts here in destructive way, hiding the oscillating information contained into the MFPT output, as we will present later on (see in Fig. 8).

Figure 3 shows the standard deviation σ (left panel), the mean velocity (center), and the mean elongation d_{med} of the monomers with respect the rest distance d_0 during the dynamics (right). d_{med} is calculated as the mean along the chain of the distance between subsequent monomers, then further averaged in the number experiments. The negative values of d_{med} mean that the springs are in average compressed. The oscillation appears both in the mean velocity and in the elongation. The minimum passage time is obtained for the maximum velocity which also corresponds to the minimum elongation of the springs, i.e., the maximum average compression.

The computed value of τ has been averaged over the initial phase ϕ. In the low frequency limit we can compute the MFPT value as

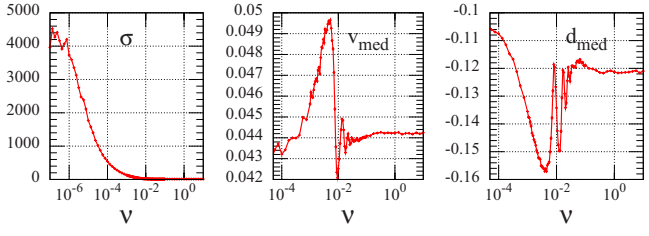

FIG. 3. (Color online) Standard deviation σ (left), mean velocity (center), and mean difference between the rest distance d_0 and the distance of the monomers during the dynamics (right) related to Fig. 2. The negative values of d_{med} means that the springs are compressed. The oscillation appears in both the mean velocity and the elongation difference.

$$\tau_M = \frac{1}{2\pi}\int_0^{2\pi} \tau_s(\phi)d\phi. \quad (4)$$

Here τ_s is the value of the MFPT in the case of fixed potential, being the low frequency limit an asymptotic limit where the time scale of the dynamics is much faster than the period $T=1/\nu$ of the external force. In that case, the polymer "sees" a static potential in all his translocation time. Because the sliding is very slow when the force is close to zero ($\phi=0$, free diffusion case), the MFPT tends to grow up and this explains its high values.

In opposite way, the high frequency limit corresponds to a dynamical translocation scale much slower than the period T. In that case the polymer sees a constant mean force F_0, being the cosine contribution averaged to zero during the slow dynamics. In this case the MFPT can be easily evaluated analytically,

$$v_{cm}(t) = \frac{n_\gamma F_0}{N\gamma}(1 - e^{-\gamma t}) \quad (5)$$

where n_γ is the mean number of monomers at a given γ inside the force region at the high frequency limit. Integrating Eq. (5) in time we get

$$L_{cm}(\tau) = \frac{n_\gamma F_0}{N\gamma}\left[\tau + \frac{1}{\gamma}(e^{-\gamma\tau} - 1)\right], \quad (6)$$

which is the distance covered by the polymer center of mass in the time τ. Unfortunately the equation is transcendent, and the number n_γ cannot be guessed in advance. In the overdamped case ($\gamma\to\infty$) with also the related time rescaling ($\tau' = \tau/\gamma$), the equation becomes

$$L_{cm}(\tau') = \frac{n_\gamma F_0}{N}\tau'. \quad (7)$$

A rough estimation of τ' can be obtained using the rest value for the number of monomers into the field, $n_\gamma=5.5$ and L_{cm} as the distance between the initial position of the polymer center of mass $[x_{cm}(0)=-L_{cm}]$ and the position $x=0$ of the boundary. Remembering the initial condition, $L_{cm}=(N-1)/2=5.5$, we have, finally

$$\tau' = \frac{N(N-1)}{2n_\gamma F_0} \simeq 120, \quad (8)$$

which is quite close to the high frequency value of Fig. 6, where the overdamped limit is plotted together with other curves.

The intermediate region is characterized by a translocation time of the same order of magnitude than the period of the external force, $\tau\sim T$. In this special case the polymer can, in average, reach the boundary during the first period of the driving. Thus the interplay between the sliding down time and the external force period reaches its maximum synchronization at this frequency ν_m. The second minimum is reached when the polymer escapes during the second period of the driving and so on. This explains why the effect is a classical and not noise induced: the synchronization with the force driving occurs when the boundary is reached at the proper time, and this can also occur without any fluctuations, though the latter are unavoidable in the dynamics.

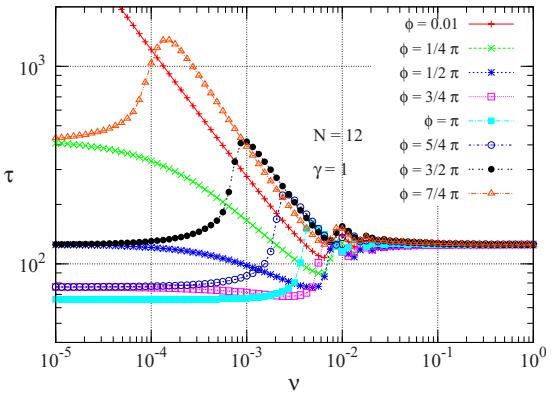

FIG. 4. (Color online) Mean first passage time τ as a function of frequency of the oscillating force for the damping parameter $\gamma=1$ with various values of the initial phase ϕ, namely, $\phi=0.01, \pi/4, \pi/2, 3\pi/4, 5\pi/4, 3\pi/2, 7\pi/4$. A minimum is always present. Moreover a very strong oscillating behavior appears in the region before the high frequency saturation value. The thermal noise intensity is $D=0.01$.

For a deeper understanding of the basic dynamics, a set of simulations have been done by fixing the initial phase, reported in Fig. 4. We can see that the MFPT can show as well a nonmonotonic behavior, depending on the ϕ value. According with the previous comments, for low frequency values, we observe very high τ values for $\phi=0.01$ (very small force during all the dynamics), while for high frequency values again the static mean force F_0 contributes to the dynamic, giving the same τ value for all the different initial phases, which is also the value of the randomly chosen initial conditions. The intermediate region shows first minima or first maxima at different positions, depending on increasing or decreasing initial forces, respectively, followed again by oscillations. It is worth to note that the couple of opposite initial phases ($\phi=\pi/4$ and $\phi=5\pi/4$, or $\phi=3\pi/4$ and $\phi=7\pi/4$) show the same τ value in the low frequency limit, because the force is the same nevertheless the direction (upward or downward) of the cosine function is, and for the couple $\phi=\pi/2$ and $\phi=3\pi/2$ this limit is the same of the high frequency one, because the limit force is F_0 in both cases.

As we mentioned previously, τ_m, the first minimum of the MFPT versus frequency curve, which is also the global minimum, satisfies a very robust relation with the period of the driving for this minimum, T_m, given by

$$1/\nu_m = T_m = \alpha\tau_m, \quad (9)$$

were $\alpha=1.36\pm0.02$ (see Fig. 5). This means that the minimum translocation time is obtained for a driving period which approximately corresponds to one and one third the time the polymer takes to cross the boundary. The above condition has been checked for all the values of γ and all the polymer length we have studied.

As a further confirmation of Eq. (9), we show in Fig. 6 the oscillating MFPT region for different values of damping. In

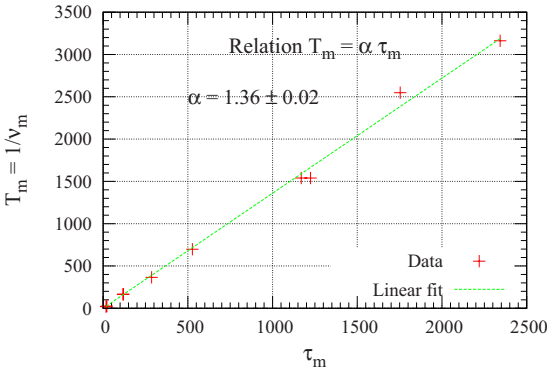

FIG. 5. (Color online) Resonant MFPT (τ_m) vs resonant period (T_m) for all the case investigated. The data concerns the parameters γ=0.01,0.1,1,10,15,20 and also the overdamped case with N=12. Furthermore, for γ=1, the different polymer length N=12,18,24,36. All the points lie on the linear relation given by Eq. (9).

order to compare the curves, the MFPT and the frequency have been scaled by damping. The presence of a minimum followed by a series of oscillations is observed for all the values of the damping. In fact, by diminishing the damping we obtain higher τ/γ ratios but the scaled position of the minima and the amplitude of the oscillations do not change. It shows that the robustness of the oscillating pattern goes beyond Eq. (9).

Further, the presence of the fluctuations with different damping at the same amplitudes (in the scaled values), demonstrate once more that the oscillating behavior has nothing to do with inertial features and inner vibrational chain modes, as one can infer at a first look of the affect.

A. Length scaling

Based on the hypothesis that in a polymer the friction is proportional to L^{μ}, for the driving case it has been proposed [9] that the translocation time of a polymer follows a scaling

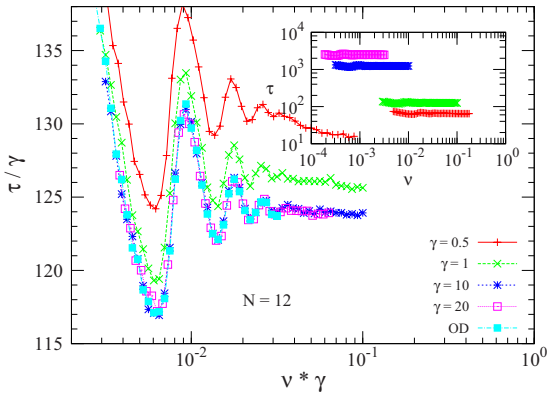

FIG. 6. (Color online) The minimum and the oscillating behavior is present independently on the damping parameter γ. The figure shows the calculations for different γ values: 0.5, 1, 10, 20, plotted following the scaling indicated in the legend of the axis. γ=10 approaches very well the overdamped limit (also shown). In the inset we show the curves without scaling.

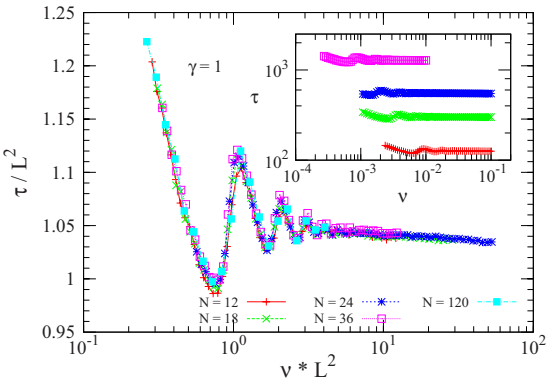

FIG. 7. (Color online) MFPT as a function of ν for different values of the polymer length L, namely N=12, 18, 24, 36, and 120. When axis is properly scaled all the original curves (shown in the inset) superimpose upon each other.

law with respect to its length L as $\tau \propto L^{1+\mu}$, where μ is a certain constant. This doubtful dependence has been recently discussed in Ref. [10,11].

In our unidimensional case the scaling law we recover appears to be in good agreement with the Rouse prediction [8,12]

$$\tau \propto L^2. \tag{10}$$

Figure 7 shows that the scaling properties hold here in a precise way. There we show our numeric results for five different polymer size, N=12,18,24,36,120. It is observed that the translocation times follow perfectly the scaling law $\tau \propto (N-1)^2$ where $N-1$ is proportional to the total length: $L=d_0(N-1)$ with d_0 the rest distance between two subsequent monomers. This relation confirms again the robustness of Eq. (9). The scaling law given in Eq. (10) has been also proved by other works where a constant force was used to drive the polymer translocation in a 1d case [10,13].

B. Thermal noise contribution

The oscillating behavior depends on the thermal noise in a destructive way. As we can see in Fig. 8, the role of the thermal noise then appears to be to destroy the oscillations. These are present in the classical dynamics (no noise, only random initial phase), but the number of visible maxima decreases by increasing the noise intensity, and the value of its maxima decreases monotonically. Only the first maximum remains barely visible in the plot at the highest temperature values there shown. It has to be observed that the behavior shown in Fig. 8 for high values of D, is qualitatively the same of the typical resonant activation (RA) phenomenon [7], where a particle overcomes a potential barrier. RA effect has been observed also in polymer dynamics [14] with a characteristic curve very similar to the behavior shown here. In this sense an experimental curveshowing similar behavior as a function of the frequency to the one here described, can be related to the presence of a fluctuating barrier or, as in the case here presented, to an oscillating linear driving in a high temperature environment.

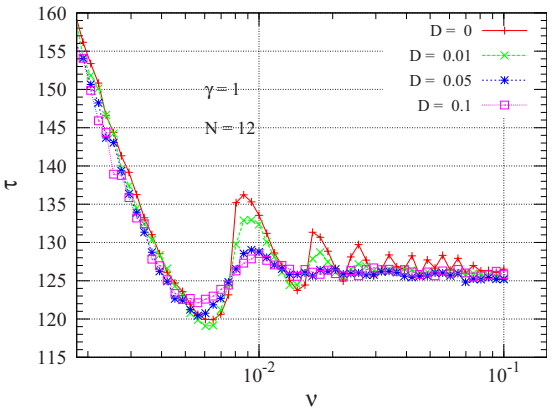

FIG. 8. (Color online) Range of the oscillating effect for different thermal noise intensity, namely: $D=0,0.1,0.5,0.1$. The oscillating behavior tends to disappear by increasing the temperature. The maxima decrease and the minima increase.

C. Stall force

A last result of the model here studied, useful for future analysis and comparisons with other models or experimental outcomes, is the evaluation of the stall force, i.e., the force necessary to stop the polymer translocation. In order to do that, a set of simulation have been performed by applying a pulling force F_p (See Fig. 9) on the left side of the chain. The initial condition has been fixed now with the polymer center of mass in the center of the external potential, and the velocity of the center of mass is measured waiting for the exit on the left or on the right of the potential region. A zero mean velocity allows to estimate the stall force of the system.

As it is visible in the inset of Fig. 7, the mean velocity of the polymer shows a strong oscillating behavior, similar for all the γ values here used. Surprisingly, the oscillations are not always present in the velocity used for the stall force evaluation. In fact for $\gamma=0.1$ they are present, while for $\gamma=1$ they are not. The inset of the two Figs. 10 and 11 show the two cases. Similarly the two related stall forces present different behavior. With two minima the one with $\gamma=0.1$ (Fig. 10), with only one the other with $\gamma=1$ (Fig. 11).

In both cases a strong mean frequency dependence of the stall force is depicted, though the intensity of force variation appears relatively not very high. In fact the variation in the scale is somehow small, and an experimental verification could be not immediately simple to perform. In this sense the more realistic model depicted in [16] is much more checkable.

IV. CONCLUSIONS

We have studied the main characteristics of a simple toy model for studying the translocation time of a polymer

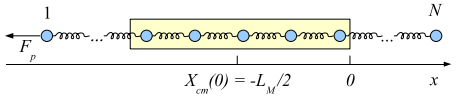

FIG. 9. (Color online) A force pull is applied at the first monomer to measure the stall force of the potential.

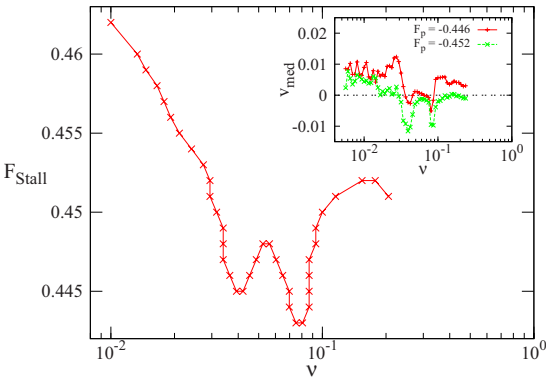

FIG. 10. (Color online) Stall force as a function of the frequency of the oscillating driving for $\gamma=0.1$. The other parameters are the same of Fig. 7. The inset shows the mean velocity versus frequency curves for two values of the pull force, $F_p=-0.446$ and -0.452.

driven by a uniform force oscillating sinusoidally in time and acting on a limited spatial region. The translocation time, as well as the stall force of the system, shows a strong dependence on the frequency of the driving. This dependence is visually similar, in many respects, and with many *distinguo*, to the resonant activation phenomenon. The driving frequency for the minimum translocation time follows with strict proportionality the computed value of this very time. A simple scaling law for the polymer length, $\tau \propto L^2$ has been found. The role of the noise intensity has been also investigated, which gives, in this case, destructive effects on the registered MFPT oscillating behavior. Finally, we have studied the stall force of the motor as a function of the driving frequency, finding a clear nonmonotonic behavior.

We present here results for a one-dimensional model. Further investigations will consider dimensionality effects on the quantities here calculated. Dimensionality could be irrelevant for polymers constrained to move in confined channels. Moreover, in many experimental situation the polymer

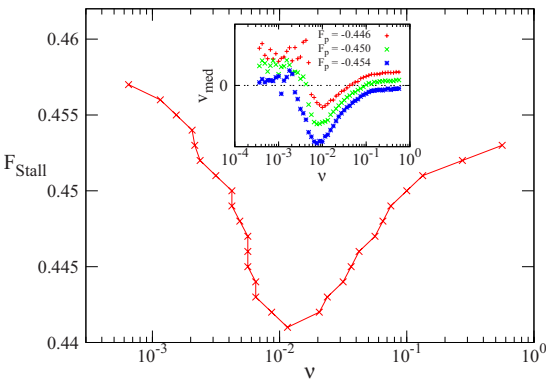

FIG. 11. (Color online) Stall force as a function of the frequency of the oscillating driving for $\gamma=1$. The two minima displayed in Fig. 10 have disappeared, and now only a minimum appears. The other parameters are the same of Fig. 7. The inset shows the mean velocity versus frequency curves for three values of the pull force, $F_p=-0.446$, -0.450, and -0.454.

is stretched, thus removing the dimensionality dependence of the measured quantities.

The model can have artificial application in nanotechnological devices driven by oscillating fields, and represents a first step to further analysis and applications to realistic biological translocation processes.

ACKNOWLEDGMENT

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