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Reversals of noise induced flow

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Abstract

We consider diffusive motion on a periodic, anisotropic potential. Adding a zero-average force that fluctuates between three values: $-F$, 0 and $+F$, can bring about net flow. As the frequency of the fluctuations varies the direction of the flux can change. We discuss a possible application for the construction of a device to separate macromolecules.

1. Introduction

A periodic potential is fluctuating between three profiles as in Fig. 1. In state 0 there is a periodic anisotropic piecewise linear profile and no net force, in the + state there is an added force to the left (i.e. a potential with a positive slope) and in the − state the same force is added to the right (i.e. a negatively sloped potential). So, basically, we have the profile of the 0 state and added noise in the form of a force that is fluctuating in a Markovian fashion between $-F$, 0 and F. We consider the behavior of a Brownian particle in this system.

In the treatment that follows we take F, E and α such that the potential is monotonically going up in the − state and monotonically going down in the + state ($F \gg E/\alpha$ and $F \gg E/(1-\alpha)$). More specific conditions allow for approximations that will be formulated later.

It is known that dichotomous zero-average fluctuating forces super-imposed on an anisotropic periodic potential can bring about a net flux [1]. It is understood how and in what direction flux occurs and how this flux changes are the flipping rate changes. Here we go beyond the dichotomous noise that Magnasco studied in Ref. [1] but, unlike Doering et al. [2], we stay in a realm that is analytically managable by a computer algebra system like "Mathematica". In the next three sections it will be observed how the induced flux changes as the correlation time of the noise changes. Because our noise is three-state we can vary another parameter, the flatness, which reflects how much time is spent in the 0-state versus the + and − states. The dichotomous noise of Magnasco in Ref. [1] has a flatness of one, which cannot be varied. We will also observe how the flux varies as a function of the flatness. For different domains in the parameter space we can qualitatively understand how and why flux and reversals of flux occur. We can, moreover, construct approximations for how the flux changes when characteristics of the noise are changed.

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2. Low frequency domain

The low frequency limit is when $\log \gamma \to -\infty$. In the low frequency domain there is, in each of the three states, enough time for the probability distribution to relax to and spend most of the time in the stationary probability distribution belonging to that state. For large enough E $(E > 4)$ the probability distribution in the 0 state can be approximated by Delta functions at $\ldots, -1, 0, 1, 2, \ldots$.

In the 0 state the net flux $J(0)$ is zero. The flux in the $-$ state is $J(-F)$ and the flux in the $+$ state is $J(F)$. The fluxes $J(-F)$ and $J(F)$ can be explicitly evaluated in this adiabatic limit (cf. Ref. [1]). Of the four slopes involved in the $+$ and $-$ state, with $\frac{1}{2} < \alpha < 1$ the $(-E/(1-\alpha)+F)$ slope of the $+$ state is the smallest. One can think of this slope as the bottleneck and the reason that we get $|J(-F))| > |J(F)|$ in the low frequency limit. We thus have a net flow to the right (i.e. a positive flux) in the low frequency limit.

Increasing γ away from the low frequency limit another effect, giving flux to the left, starts to play a role. Provided γ is small enough, we get, in the $+$ and $-$ states, a spread of the probability where a fraction α is in the intervals $\langle k, \alpha+k \rangle$ and a fraction $1-\alpha$ is in the intervals $\langle \alpha+k, k+1 \rangle$, where k is any integer. So more probability ends up on the long slope than ends up on the short slope. If, in that case, we flip to the 0 state and go back to the delta functions at $-1, 0, 1, 2, \ldots$, there will be a shift to the left of the center of mass of $\alpha - \frac{1}{2}$. We will call this the "flashing barrier" effect.

Next we will use these ideas as a basis for a quantitative approximation. In Fig. 2 τ_- is the fraction of time spent by the potential in the $-$ state, likewise, τ_+ is the fraction of time spent in the $+$ state and τ_0 is the fraction of time spent in the 0 state (see Fig. 2).

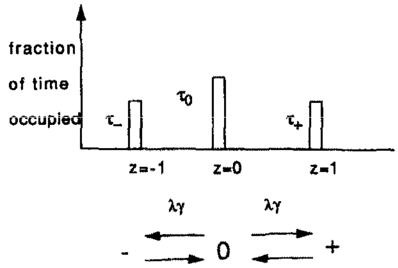

Fig. 2. The variable κ in the kinetic scheme determines the fractions of time spent in the $+$, 0 and $-$ states.

From the equations

$$\tau_- + \tau_0 + \tau_+ = 1, \quad \tau_- + \tau_+, \quad \lambda\tau_0 = \tau_+,$$

we obtain $\tau_- = \tau_+ = 1/(2- +1/\lambda)$ and also the "flatness", the ratio of the fourth moment and the square of the second moment, is easily obtained,

$$\varphi = \frac{\langle z^4 \rangle}{\langle z^2 \rangle^2} = \frac{\tau_+ + \tau_-}{(\tau_+ + \tau_-)^2} = \frac{1}{\tau_+ + \tau_-} = \frac{1}{2\tau_-}$$

$$= \frac{1}{2\tau_+} = 1 + \frac{1}{2\lambda}.$$

In the low frequency limit the net flux is

$$\tau_- J(-F) + \tau_+ J(F) = \frac{1}{2\varphi}\left[J(-F) + J(F)\right].$$

The average number of transitions per unit of time into the "0" state is $(\tau_- + \tau_+)\gamma = \gamma/\varphi$ and we thus obtain as the linear approximation at low frequency

$$J(\gamma) = \frac{1}{\varphi}\left\{\tfrac{1}{2}\left[J(-F) + J(F)\right] - \left(\alpha - \tfrac{1}{2}\right)\gamma\right\}.$$

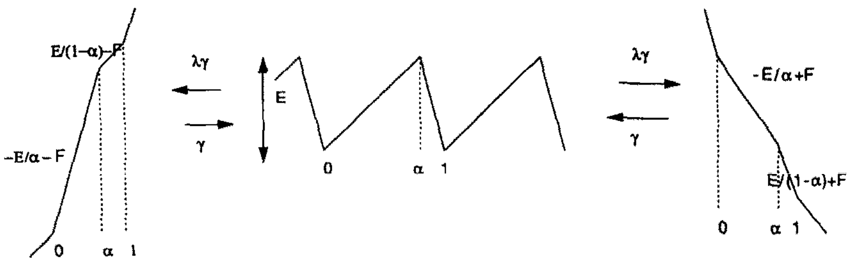

Fig. 1. The setup for the system. The periodic, anisotropic potential is shown in the middle. A macroscopic force that fluctuates between $-F$, 0 and $+F$, where F is large, is applied and leads to the system fluctuating between the three depicted profiles.

To get an idea until what γ this approximation is valid we perform the following calculation. We take for the diffusion coefficient $D = 1$ and take as the unit of length the period of the potential. In the + or − state, with at $t = 0$ a Dirac delta function at $x = 0$, we get a spreading Gaussian as time evolves,

$$P(0, x; t) \approx \frac{1}{2\sqrt{\pi t}} \exp\left(- \frac{(x \pm Ft)^2}{4t} \right).$$

We see that after $\frac{1}{8}$ a unit of time (i.e. $\gamma = 8$ so $\log \gamma \approx 1$) the standard deviation around $\frac{1}{8}F$ is half a period.

For a large enough positive F we can take $\sinh(\frac{1}{2}F) \approx \cosh(\frac{1}{2}F) \approx \frac{1}{2}e^{F/2}$ and for large enough negative F we have $\sinh(\frac{1}{2}F) \approx \cosh(\frac{1}{2}F) \approx \frac{1}{2}e^{-F/2}$. Substituting this in Magnasco's [1] formulae for $J(F)$ and $J(-F)$, we find that all the exponentials cancel. When we moreover have $E^2/F^3 \ll \alpha^2(1-\alpha)^2$ we can make some neglections and find

$$J(F) + J(-F) \approx F\left(\frac{(\alpha - E/F)(1 - \alpha + E/F)}{\alpha(1-\alpha) + (2\alpha - 1)E/F} - \frac{(\alpha + E/F)(1 - \alpha - E/F)}{\alpha(1-\alpha) - (2\alpha - 1)E/F} \right).$$

Expanding this expression in powers of E/F we find that the first nonzero term occurs at third order, whence we get the approximation

$$J(F) + J(-F) \approx \frac{2F(2\alpha - 1)}{\alpha^2(1-\alpha)^2} \left(\frac{E}{F} \right)^3.$$

For the flux J as a function of the flipping rate γ we end up with the following relatively simple approximation for the low frequency domain,

$$J(\gamma) \approx \frac{1}{\varphi} \left(\frac{(2\alpha - 1)E^3}{\alpha^2(1-\alpha)^2 F^2} - (\alpha - \tfrac{1}{2})\gamma \right).$$

In Fig. 3 this approximation (the dotted line on the left) is graphed together with the exact evaluation (the solid line) for $F = 200$, $E = 8$, $\lambda = 1$ (which implies $\varphi = \frac{3}{2}$ and $\alpha = \frac{7}{8}$. The exact evaluation can be obtained following the method described in Ref. [3]. The difference with the dichotomous case is that here we face three coupled second order linear homogeneous equations. So the exponents have to be obtained from an eigenvalue equation which is a fifth order polynomial and the coefficients follow from a linear algebraic system of twelve equations.

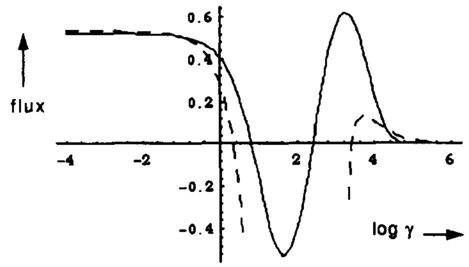

Fig. 3. The solid line gives the flux as a function of the flipping rate γ for the system shown in Fig. 1. The parameter values are $E = 8$, $F = 200$, $\alpha = \frac{7}{8}$ and $\lambda = 1$ (leading to a flatness of $\varphi = \frac{3}{2}$). The dashed line on the left is the result of the low frequency approximation and the dashed line on the right is the result of the high frequency approximation.

We see that the approximation does indeed work well until about $\log \gamma \approx 1$. It appears furthermore that the approximation does cover the first flux reversal and that the "flashing barrier" effect is indeed "responsible" for this flux reversal. Finally, it is interesting to note that the frequency at which the first flux reversal takes place is, in the linear approximation, independent of the flatness of the noise.

3. High frequency domain

In the high frequency limit we take as a starting point the probability density distribution on the average potential and we calculate how this Boltzmann distribution gets "jolted" by the fluctuating force. The average potential is the 0 state. We normalize the probability over one period. For a sufficiently large value of E (such that we can neglect e^{-E} relative to 1) the normalization factor approximates E and with the energy in units of kT we have

$$p(x) = p_1(x) = Ee^{-Ex/\alpha} \quad \text{if } 0 \leqslant x \leqslant \alpha,$$
$$= p_2(x) = Ee^{-E(1-\alpha)/(1-x)} \quad \text{if } \alpha \leqslant x \leqslant 1.$$

It is the barrier at $x = \alpha$ that is the bottleneck for the flux. In the 0 state there are not very many "jumps" over this barrier and, moreover, there are as many forward as backward ones. Net flux occurs because in the + state there is a different probability for a

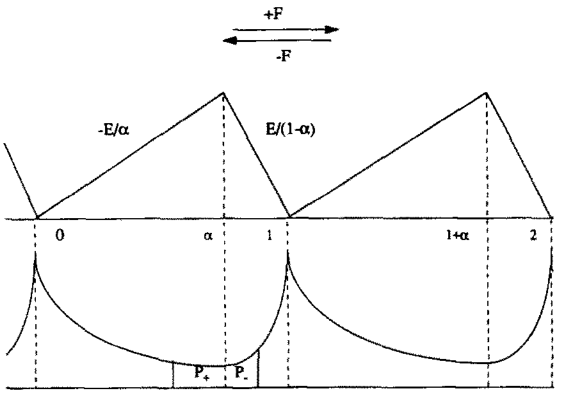

Fig. 4. The basic idea behind the high frequency approximation. The top shows the average potential and the bottom shows the Boltzmann distribution on this potential. During a sojourn in the $+F$ state an amount of probability P_+ is pushed over the barrier in the positive direction and during a sojourn in the $-F$ state an amount P_- is pushed over the barrier in the negative direction. For small dwelling times $P_+ > P_-$, because the $(\alpha, 1)$ slope is steeper than the $(0, \alpha)$ slope. But for larger dwelling the faster increase of P_- away from α leads to $P_- > P_+$.

forward jump than there is for a backward jump in the $-$ state. Thinking of this flux as deterministic (like in hydrodynamics) will help us to understand the flux as a function of γ in the high frequency domain, including the flux reversal (see Fig. 3).

Consider Fig. 4 which depicts the average potential as well as the probability density. Whenever $+F$ is "on" for $1/\gamma$ units of time an amount of probability of

$$P_+ = \int_{\alpha-(-E/\alpha+F)/\gamma}^{\alpha} p_1(x)\, \mathrm{d}x$$

is pushed forward over the barrier. When $-F$ is "on" for $1/\gamma$ units of time an amount

$$P_- = \int_{\alpha}^{\alpha+[1-E/(1-\alpha)+F]/\gamma} p_2(x)\, \mathrm{d}x$$

is pushed backward over the barrier. The areas P_+ and P_- are indicated in Fig. 4. It is easy to see that for very high γ the width of the areas P_+ and P_- goes to zero and we can approximate: $P_+ \approx p_1(\alpha)(-E/\alpha+F)/\gamma$ and $P_- \approx p_2(\alpha)(-E/(1-\alpha)+F)/\gamma$. Here $(-E/\alpha+F)/\gamma$ is the width of area P_+ and $[-E/(1-\alpha)+F]/\gamma$ is the width of area P_-. We have $p_1(\alpha) = p_2(\alpha) = E\ \mathrm{e}^{-E}$. With $\frac{1}{2} < \alpha < 1$ the width of the P_+ area is bigger than that of the P_- area and thus $P_+ > P_-$. This means a flow in the positive direction for the fluctuating system as a whole. When we lower the value of γ the widths of P_+ and P_- both grow with the same factor, but the average height of the P_- area grows a lot faster than the average height of the P_+ area. This "height effect" is exponential and will in the end always "win" in comparison to the linear width effect. Around the point where $P_+ = P_-$ there is a flux reversal.

To get quantitative accuracy of our approximation and to get zero flux at $\gamma \to \infty$ we have to take one more effect into account. A particle that gets pushed a distance δ across the $x = \alpha$ barrier when $+F$ is "on" has a probability of $(\mathrm{e}^{E}\mathrm{e}^{-E\,\delta/(1-\alpha)} - 1)/(\mathrm{e}^{E} - 1)$ to go back over the barrier and get back to the trench it came from when the system is again in state 0 (see Ref. [4], Section 5.2.8). For a particle that gets pushed a distance ε in the negative direction by $-F$ this return probability equals $(\mathrm{e}^{E}\mathrm{e}^{-E\,\varepsilon/\alpha} - 1)/(\mathrm{e}^{E} - 1)$. For $\gamma \to \infty$ the distances δ and ε get very small and the return probabilities approach one.

Next we take all the abovementioned effects into account and obtain one expression for the flux as a function of $\log \gamma$ to approximate the high frequency domain. A particle at location x in the P_+ area is at x' after application of $+F$ for $1/\gamma$ units of time (remember: we neglect diffusive effects). We have for the relation between x and x',

$$x' = \alpha + \left(\frac{1}{\gamma} - \frac{\alpha - x}{-E/\alpha + F}\right)\left(\frac{E}{1-\alpha} + F\right).$$

The amount of probability that eventually gets transferred by "one trench" (i.e. one period = one unit of distance) by $+F$ applied for $1/\gamma$ units of time is

$$R_+ = \int_{x'=\alpha}^{\alpha+[E/(1-\alpha)+F]/\gamma} p_1(x)\,\pi^{(1)}(x')\, \mathrm{d}x',$$

where $\pi^{(1)}(x')$ is the probability that a particle that mounts the $x = \alpha$ barrier when $+F$ is "on" actually goes on to $x = 1$ (versus diffusing back over the barrier) when $+F$ is "off" again. We have (cf. Ref. [4], Section 5.2.8)

$$\pi^{(1)}(x) = \frac{\mathrm{e}^{E} - \mathrm{e}^{E(1-x)/(1-\alpha)}}{\mathrm{e}^{E} - 1}.$$

Likewise we have

$$R_- = \int_{x'=\alpha-(E/\alpha+F)/\gamma}^{\alpha} p_2(x)\pi^{(0)}(x')\,\mathrm{d}x',$$

with

$$\pi^{(0)}(x) = \frac{\mathrm{e}^E - \mathrm{e}^{E_x/\alpha}}{\mathrm{e}^E - 1}.$$

The integrals can be evaluated analytically by "Mathematica" and the net flow of the fluctuating system is $J = \gamma(R_+ - R_-)/2\varphi$. The result of this approximation for $F = 200$, $E = 8$, $\alpha = \frac{7}{8}$ and $\varphi = \frac{3}{2}$ is the dotted line on the right edge of Fig. 3. The approximation is no longer useful at flipping times larger than about 5×10^{-4}, i.e. $\log \gamma < 3.3$, because this is about the time it takes to slide down the short slope when "$+F$" is on. For longer flipping times the areas P_+ and P_- start to extend over several periods which would lead to complicated expressions (sums of integrals) for R_+ and R_-.

Though the approximation has the right shape, its peak occurs at a value that is a factor 5 lower than the real solution. The flux reversal in the approximation takes place at a value for the flipping rate that is a factor 5 too high. There are many effects that ought to be taken into account for quantitative accuracy. We neglected, for instance, diffusive forces. We also took the average transferred areas P_+ and P_- to be the areas transferred during an average dwelling in the + and − state.

4. Flux reversals

When the flatness is increased from its minimum value of 1 to ∞, the fraction of time spent in the 0 state grows from 0 to 1. For a flatness of 1 we have the dichotomous noise that was studied by Magnasco in Ref. [1]. In that case (see Fig. 5a) we have no flux reversals and for increasing $\log \gamma$ the flow decreases sigmoidally and monotonically to 0. Taking values of the flatness away from 1 (see Fig. 5b) we create the discussed "flashing barrier" effect. In a flux versus $\log \gamma$ graph this effect translates into a dip at at around $\log \gamma = 1.5$.

In the high frequency domain Figs. 5c and 5d

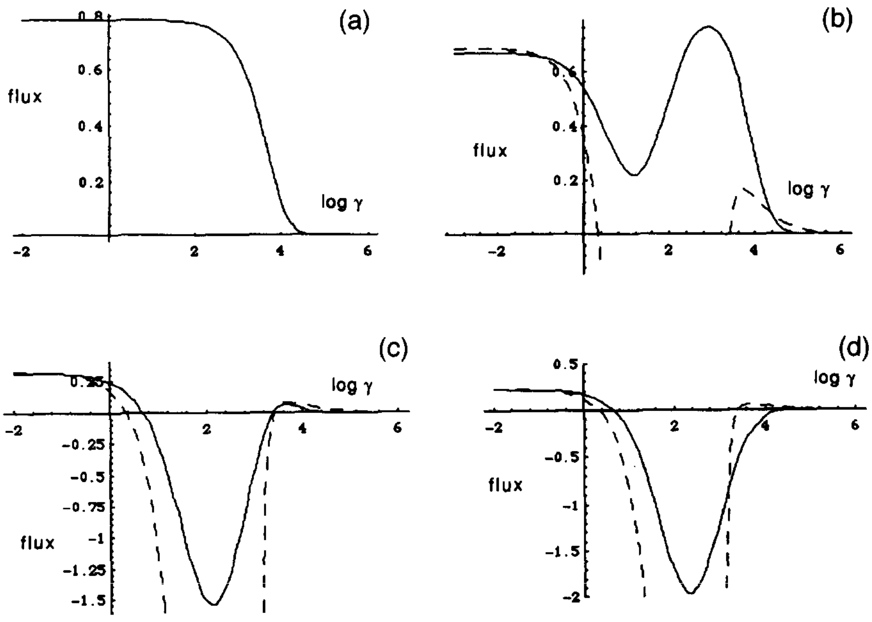

Fig. 5. The flux as a function of the flipping rate γ for $E = 8$, $F = 200$, $\alpha = \frac{7}{8}$ and different values of the flatness: (a) $\varphi = 1$, (b) $\varphi = \frac{7}{6}$, (c) $\varphi = \frac{5}{2}$, (d) $\varphi = \frac{7}{2}$. The dashed lines again indicate the low and high frequency approximations. No flux reversals occur when the flatness is too close to one. Beyond a certain critical flatness around 3 the last flux reversal no longer occurs and $J = 0$ is approached from the negative side.

show that the last flux reversal is no longer present at a sufficiently high flatness; $J=0$ appears to be approached from above when $\varphi=2.5$ and from below when $\varphi=3.5$. This behavior is not reflected in the high frequency approximation described in the previous section. Elston and Doering have carried out an asymptotic expansion of the flux J in powers of $1/\gamma$ [5]. Their analysis is for a general potential $\upsilon(x)$ with period 1. The first nonzero term in the expansion appears at third order in $1/\gamma$,

$$J=\frac{1}{ZY}\left(\frac{F^4(\varphi^2-3\varphi+1)}{\varphi^3}\int_0^1\nu'(x)^3\,\mathrm{d}x\right.$$
$$\left.-\frac{F^2}{\varphi}\int_0^1\nu'(x)[\nu''(x)]^2\,\mathrm{d}x\right)(1/\gamma)^3$$
$$+\,\mathrm{O}\big((1/\gamma)^4\big),$$

where $Z=\int_0^1\exp[-\nu(x)]\,\mathrm{d}x$ and $Y=\int_0^1\exp[\nu(x)]\,\mathrm{d}x$. For large values of F, such as the one we have used in our examples, the first term which goes with F^4 is expected to dominate over the second F^2 term. The first term indeed switches sign at $\varphi=\frac{1}{2}(3+\sqrt{5})=2.62$ and this seems consistent with our observations. The first term of the expression generally fits the exact solution very well for different values of the flatness when $\log\gamma>4$. The problem is that the formula of Elston and Doering is for smooth potentials and is not supposed to apply to our case. For our case the integral in the second term is underfined (divergent). That just the first term gives a good approximation to the exact solution is something that, for the time being, we must accept as a "happy coincidence" and might be better understood once we have a complete expansion.

5. Discussion

That nonequilibrium fluctuations can bring about flux has been known for a while [6]. What we have shown and explained in this paper is that the direction of the induced flux can depend on characteristics of the noise like the fastness and the flatness. It is surprising that already the relatively simple setup presented in Section 1 and Fig. 1 can lead to such rich and complicated behavior.

Systems similar to ours have been studied. Doering et al. [2] looked at the limit of infinitely fast noise with a continuous spectrum instead of three states and they varied the strength of this noise. In our notation varying the strength of the noise would mean changing F. The behavior in the high frequency realm for increasing F would be the same as for increasing dwelling times $1/\gamma$; in both cases such an increase means wider strips, P_+ and P_-, in Fig. 4. Where we took Markovian noise, Bartussek et al. [7] took a function $F(t)=A\sin(\omega t)$ (which has a flatness of $\frac{3}{2}$) and superimposed it, not on a sawtooth, but on a smooth anisotropic function. They varied the strength A, the fastness ω and the thermal noise strength (equivalent to the temperature) and found flux reversals as these parameters were changed. The behavior for piecewise linear potentials and for smooth potentials is not expected to differ much; systems with diffusion tend to be very "forgiving" to corners.

A possible application of the flux reversals could be for the separation of macromolecules. How this application arises becomes clear when we redimensionalize the variables. To unscale the frequencies (flipping rates) they have to be multiplied with $kT/\beta L^2$. The quantity β, representing the coefficient of viscous friction, is specific for each macromolecule and depends on shape and size. Different macromolecules thus "feel" a different part of the frequency spectrum.

A nanotechnological device that employs Brownian motion in the presence of a fluctuating potential to drive microscopically small particles has already been constructed by Rousselet et al. [8]. A device that operates according to the model that we have presented here would have a great advantage over any existing device. With our procedure it is always possible to find some flipping rate for which a molecule with friction β_1 moves in a direction opposite to the one of a molecule with friction β_2. Looking in Fig. 3 around $\log\gamma=2.5$ we see that a difference of a factor 10 in the viscous friction β can translate in the difference between maximum positive flow and maximum negative flow. Devices for the separation of macromolecules usually operate based on the fact that molecules with a larger β move slower in a certain direction when a force is applied in that direction. Also the fluctuating potential apparatus of Ajdari and Prost [9] makes molecules move in the same direction but at different speeds. The fluctuating force device proposed here is actually able to let molecules with different β's move in opposite directions.

Acknowledgement

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