

Reply to the comment on 'Anomalous dynamics of unbiased polymer translocation through a narrow pore' and other recent papers by D Panja, G Barkema and R Ball

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REPLY

Reply to the comment on ‘Anomalous dynamics of unbiased polymer translocation through a narrow pore’ and other recent papers by D Panja, G Barkema and R Ball

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Abstract

We reply to the comment made by Dubbeldam *et al* (2009 *J. Phys.: Condens. Matter* **21** 098001) on our paper ‘Anomalous dynamics of unbiased polymer translocation through a narrow pore’ and our other recent papers.

The comment of Dubbeldam *et al* starts with a summary of our theoretical interpretation of the problem of unbiased translocation through a narrow pore in a membrane. Their summary of our theory, except for some crucial details discussed below, is correct.

- The authors of the comment state ‘the membrane is present only as an imaginary separating plane between the left (cis) and right (trans) semi-spaces’. This statement is not correct. In all our simulations, the membrane is an impenetrable plane (excepting the pore), given by the equation $z = 0$. Denoting the monomer number in the pore as $s(t)$ at time t , all monomers $i < s(t)$ have $z_i < 0$ and all monomers $i > s(t)$ have $z_i > 0 \forall t$.
- The authors of the comment state ‘we recall here the seminal paper of Chuang *et al* where it was argued that despite $\tau_d > \tau_R$, the translocation time τ_d should scale as $\tau_d \propto N^{1+2\nu}$, where ν is the Flory exponent for the polymer ($\nu = 0.75$ in 2D, and $\nu \approx 0.588$ in 3D). This is a misrepresentation of the work by Chuang *et al* [2]. In fact, Chuang *et al* argue that the pore-blockade time (or the dwell time) $\tau_d > \tau_R$, where τ_R is the Rouse time scaling

$\sim N^{1+2\nu}$, and *only provide numerical evidence*, based on simulations in 2D with polymer lengths of $N = 128$ or less, that τ_d scales $\sim N^{1+2\nu}$ as well; they provide no theoretical argument for why τ_d should scale $\sim N^{1+2\nu}$. With $1 + 2\nu \approx 2.18$ in 3D, it is interesting to note that reference [3] by the very authors of the comment contradicts the results of Chuang *et al* by producing $\tau_d \sim N^{2.52 \pm 0.04}$ in 3D, consistent with our prediction $\tau_d \sim N^{2+\nu} \approx N^{2.588}$ as it appears in [4, 5], the papers they criticize. Furthermore, recent 2D simulations using the (bond fluctuation) model of Chuang *et al* performed by two of us [6] show that the purported scaling $\tau_d \sim N^{1+2\nu}$ does not hold for chains longer than those simulated by Chuang *et al*.

The comment of Dubbeldam *et al* [1] then raises five issues, to which we reply in order.

(1) *The chain diffusion coefficient is much larger than that for a Rouse unconstrained chain.* Here, the authors of the comment are comparing two entirely different quantities. The chain diffusion coefficient $D_N \sim N^{-\nu}$ introduced by the authors of the comment is the squared *curvilinear*

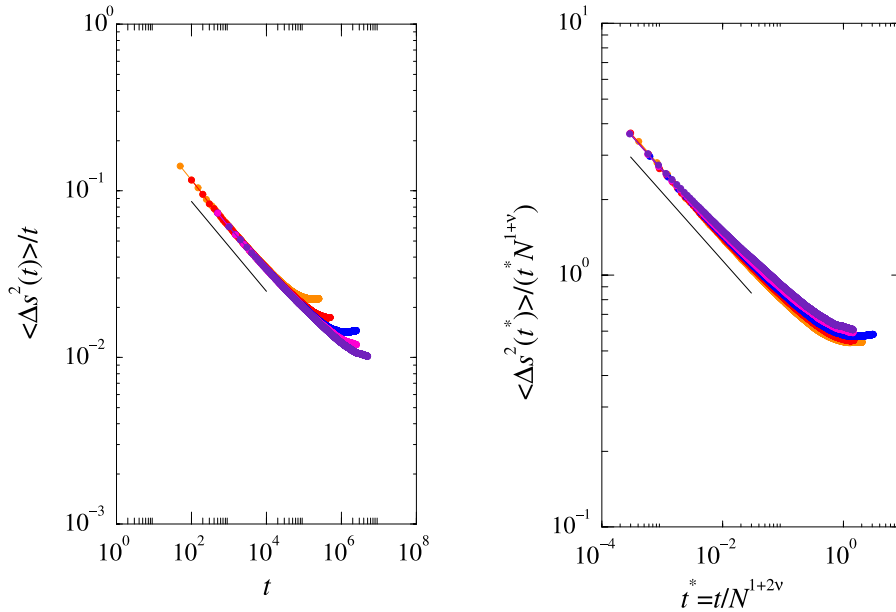


Figure 1. Left: squared translocation distance per unit of time $\langle \Delta s^2(t) \rangle / t$, as a function of t , for (from top to bottom) $N = 216$ (orange), 343 (red), 512 (blue), 729 (magenta) and 1000 (indigo). At short times, the diffusion is anomalous: $\langle \Delta s^2(t) \rangle \sim t^{(1+\nu)/(2+\nu)} \approx t^{0.73}$ in 3D [4, 5], hence $\langle \Delta s^2(t) \rangle / t \sim t^{-0.27}$ as shown by the straight black line. At long times, the diffusion behaviour crosses over to normal diffusion (curves becoming horizontal). The crossover time increases with N . Right: the same data are plotted in modified coordinates with a reasonable degree of collapse, showing that the crossover time does scale as $\tau_R \sim N^{1+2\nu}$ [4, 5]. Note that at $\langle \Delta s^2(\tau_R) \rangle \sim N^{1+\nu}$, which is used to scale the y-axis to achieve the data collapse. The straight black line again corresponds to $t^{-0.27}$.

(This figure is in colour only in the electronic version)

displacement of a tagged monomer per unit of time during the time the polymer remains threaded through the pore, whereas the Rouse diffusion coefficient is the *real-space* squared displacement of the centre of mass (or a tagged monomer) of a free polymer per unit of time. Comparing these two quantities does not make sense. We note that during the time the polymer remains threaded through the pore it is possible to convert the curvilinear displacement of a tagged monomer to its real-space displacement. The (trivial) result of this exercise is that in real space the motion of the tagged monomer remains subdiffusive as long as the polymer remains threaded through the pore, although its curvilinear motion is diffusive after the Rouse time.

A more appropriate comparison of the diffusive motion of a translocating polymer with that of a free polymer can be made by noticing that after the translocation process is finished, the centre of mass of the polymer is displaced by a distance of its own size $\sim N^\nu$ in a time $\sim N^{2+\nu}$, implying that the real-space diffusion coefficient of the centre of mass is $N^{\nu-2}$. This quantity, in the limit of large N , is less than the Rouse diffusion coefficient $1/N$, as can be clearly expected from the fact that the presence of the membrane hinders the motion of the polymer.

(2) *The existence of a crossover to normal diffusion.* Our theoretical picture is that the curvilinear squared displacement $\langle \Delta s^2(t) \rangle$ shows anomalous diffusion up to the Rouse time $\tau_R \sim N^{1+2\nu}$, after which it gradually crosses over to normal diffusion up to the unthreading time $\tau_d \sim N^{2+\nu}$, after which s is ill defined as the polymer disengages from the pore. Thus, the time range for which (normal) diffusion can be observed increases with increasing polymer length N . Clear numerical

evidence of the existence of the (normal) diffusion regime is presented in [7]. We have replotted the data in figure 1. Since this crossover is rather gradual, spanning one or two orders of magnitude in time, the diffusive regime is only clearly visible for long polymers.

(3) *Field dependence of field-driven translocation.* In our theoretical framework it is not required that the chain tension Φ at the pore (on any side of the membrane) scales linearly with the field E . It is however required that (i) $Z^{(4)}$, the centre of mass of the first four monomers on any side of the membrane, scales linearly with the chain tension Φ , as shown in figure 2 of [8] (this allows us to proxy the chain tension at the pore by $Z^{(4)}$), and that (ii) the chain tension imbalance across the pore during translocation reaches a constant fairly soon, so that the $[\phi_{t=0} - \phi(t')]$ in equation (6) of [8] can be taken out of the integral sign. For consistency with the scaling $\tau_d \sim 1/E$, it is also required that $[\phi_{t=0} - \phi(t)]$ in figure 4 of [8] should scale as $E^{(1+\nu)/(1+2\nu)} \approx E^{0.73}$ in 3D.

In figure 4 of [8] we showed that $[\phi_{t=0} - \phi(t)]$ in equation (6) does indeed go to a constant; to show this did not require extensive simulations. The data quality of that figure, however, is clearly not good enough to distinguish between $[\phi_{t=0} - \phi(t)]$ scaling as $\sim E^{0.73}$ (as it should!), as opposed to the perception of the authors of the comment that $[\phi_{t=0} - \phi(t)]$ in figure 4 of [8] scales as $\sim E$. It is nevertheless interesting to note that one of the authors of the comment (Milchev) has recently co-authored a paper [9] confirming not only our result [8] that for field-driven translocation $\tau_d \sim N^{(1+2\nu)/(1+\nu)}$, but also $\tau_d \sim 1/E$ (see figure 2 of [9]).

(4) *Nonlinear chain reaction to pulling on one end.* The authors of the comment confuse the response of the

chain to a stretching force and the response of the chain to small fluctuations in the stretching force over its pre-stretched state. The former is nonlinear—as the authors of the comment correctly state: due to the entropic repulsion between the polymer and the membrane, a translocating polymer experiences a nonlinear stretching force near the membrane. However, to first approximation, a pre-stretched chain reacts *linearly* to small fluctuations in the stretching force acting on it. Thus, the response to small fluctuations in the chain tension of a polymer over its pre-stretched state is *linear*, and this is all we need for our theoretical derivation [10].

(5) *Our earlier criticism of [3]*. The authors of the comment have totally misunderstood our criticism of their earlier work [3]. Our point is as follows. The MC simulations in [3] measured the time distribution $Q(t)$ of a process in which the initial state of the polymer is such that all of the polymer is located on the cis side of the membrane, and the final state is that all of the polymer is located on the trans side of the membrane. From this time distribution, the authors extract an average time τ , which scales as $\tau \propto N^{2.52 \pm 0.04}$. The authors of the comment argued that the ratio τ/τ_R is accounted for by an entropic barrier [3].

Suppose that the authors repeat their exercise, but now starting in an initial state in which the middle of the chain is located in the pore (i.e., *the initial state of the polymer is located at the top of the entropic barrier*), and simulate until the final state is reached, in which the polymer is either on the cis or on the trans side; resulting in an average unthreading

time τ_M . This average unthreading timescales linearly with the dwell time, i.e., $\tau_d \sim \tau_M$ [5, 11].

We have shown in [4, 5] that $\tau \sim \tau_M$; this, combined with $\tau_d \sim \tau_M$, yielded us $\tau_d \sim \tau$. These prove two points: (i) as reported in [4, 5], the timescale τ for crossing the purported entropic barrier [3] and the timescale τ_M for going downhill from the top of the entropic barrier scale linearly with each other; i.e., the entropic barrier has no influence on the pore-blockade time, contrary to the claim of [3]. (ii) Our theoretical result $\tau_d \sim N^{2+\nu} \approx N^{2.588}$ [4, 5] is in good agreement with the numerical result $\tau \sim N^{2.52 \pm 0.04}$, as reported in [3].

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