Comment on “Passage Times for Unbiased Polymer Translocation through a Narrow Pore”

Kaifu Luo,1 Tapio Ala-Nissila,1,2 See-Chen Ying,2 Pawel Pomorski,3 and Mikko Karttunen3

1Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 TKK, Espoo, Finland
2Department of Physics, Box 1843, Brown University, Providence, Rhode Island 02912-1843, USA
3Department of Applied Mathematics, The University of Western Ontario, London, Ontario, Canada

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One of the most fundamental quantities associated with polymer translocation through a nanopore is the translocation time \( \tau \) and its dependence on the chain length \( N \). In a recent Letter, Wolterink et al. [1] present new results for unbiased translocation using a 3D lattice model within the Monte Carlo (MC) simulation method. According to their scaling argument \( \tau \sim N^{1+2\nu} F(b/R_g) \), where \( R_g \) is the radius of gyration, \( b \) the pore width, the Flory exponent \( \nu = 0.75 \) in 2D and 0.588 in 3D, and numerically the scaling function \( F(x) \sim x^{-0.38 \pm 0.08} \) for \( x \to 0 \). This leads to \( \tau \sim N^{2.40 \pm 0.08} \), which is in contradiction with the established result by Chuang et al. [2] that \( \tau \sim N^{2\nu + 1} \), which gives 2.50 in 2D and 2.18 in 3D.

The original prediction that \( \tau \sim N^{2\nu + 1} \) [2] means that \( \tau \) scales with \( N \) in the same manner as the Rouse relaxation time of the chain except for a larger prefactor, \( \tau_R \sim R_g^2/D \sim N^{1+2\nu} \), where the diffusion coefficient \( D \sim 1/N \) within Rouse dynamics. This result was recently corroborated by extensive numerical simulations based on the Fluctuating Bond (FB) [3] and Langevin Dynamics (LD) models with the bead-spring approach [4,5], where \( \tau \) was found to scale as \( N^{2.50 \pm 0.01} \) in 2D.

To resolve the apparent discrepancy, we have analyzed the approach of Wolterink et al. [1] and performed additional high-accuracy numerical simulations using the FB model with MC dynamics [3] in 2D, and atomistic MD simulations using the GROMACS [6] simulation engine in 2D and 3D. As in the MC and LD methods, explicit solvent hydrodynamics were excluded in our GROMACS simulations. We find that within numerical accuracy, both the FB and MD methods give the same scaling results in 2D, and thus here we present data as obtained using GROMACS within the bead-spring model. GROMACS is currently one of the most commonly used programs in soft matter and biophysical simulations, and has also been used extensively by some of us in various problems (see e.g., Ref. [7] and references therein).

Our main results are summarized in Fig. 1, where we find that \( \tau \sim N^{2.44 \pm 0.03} \) in 2D and \( \tau \sim N^{2.22 \pm 0.06} \) in 3D in complete agreement with Refs. [3,4,5], ruling out results of Ref. [1] within the accuracy of the data. In particular, we find that the scaling function \( F(b/R_g) \) becomes independent of \( N \) for large \( N \), as shown in the insert of Fig. 1. Thus, there is no discernible correction to the exponent \( 1 + 2\nu \).

To verify our results independently, we also computed the squared change of the translocation coordinate \( s(t) \), where we observed sub-diffusive behavior \( \langle (\Delta s(t))^2 \rangle \sim t^{\alpha} \), with \( \alpha = 0.807 \pm 0.002 \) in 2D and \( \alpha = 0.910 \pm 0.002 \) in 3D. This again agrees with Chuang et al. [2] who obtained \( \alpha = 2/(1 + 2\nu) \), which gives 0.8 in 2D and 0.92 in 3D.

Further theoretical support for the exponent \( 1 + 2\nu \) comes from two other independent studies. In Ref. [3] it was analytically predicted and also numerically confirmed that \( \tau \sim (R_g + L)^2/D \) for a pore of length \( L \), resulting from the fact that the mass center of the polymer moves a distance of \( L \) in the hole. For long pore \( L \gg N \) we have \( \tau \sim NL^2 \gg N^3 \), which is longer than the reptation time of the chain \( \sim N^3 \).

In the second study a different approach was used: the starting point was driven translocation in which a pulling force \( F \) is acting on one end of the chain. In that case, \( \tau \sim N^{2\nu + 1} \) can be analytically derived in the limit \( F \to 0 \) using well-established scaling functions for polymers under tension [8].

To conclude, all the above independent results, analytical and numerical, and in particular the behavior of the scaling function \( F(b/R_g) \), confirm the result \( \tau \sim N^{2\nu + 1} \), and invalidate the lattice model results of Ref. [1]. The apparent discrepancy may be due to the artificial dynamics of the lattice model of Ref. [1], which is based on the reptating polymer model for a single reptating polymer with the addition of sideways moves and reptation moves; although their lattice model works well for static properties in bulk solutions [9], the dynamics in the presence of a narrow hole may pose problems as the hole adds a new length scale to the problem. An off-lattice approach, such as used here is guaranteed to be free of any artifacts.

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[1] J.K. Wolterink, G.T. Barkema, and D. Panja, Phys. Rev. Lett. **96**, 208301 (2006).
[2] J. Chuang, Y. Kantor, and M. Kardar, Phys. Rev. E **65**, 011802 (2001).
[3] K. Luo, T. Ala-Nissila, and S.C. Ying, J. Chem. Phys. **124**, 034714 (2006).
[4] I. Huopaniemi, K. Luo, T. Ala-Nissila, and S.-C. Ying, J. Chem. Phys. **125**, 124901 (2006).
[5] D. Wei, W. Yang, X. Jin, and Q. Liao, J. Chem. Phys. **126**, 204901 (2007).
[6] D. van der Spoel, E. Lindahl, B. Hess, G. Groenhof, A.E. Mark, and H.J.C. Berendsen, J. Comp. Chem. **26**, 1701 (2005).
[7] M. Patra, E. Salonen, E. Terama, I. Vattulainen, R. Faller, B.W. Lee, J. Holopainen, and M. Karttunen, Biophys. J. **90**, 1121 (2006).
[8] I. Huopaniemi, K. Luo, T. Ala-Nissila, and S.-C. Ying, Phys. Rev. E **75**, 061912 (2007).
[9] A. van Heukelum and G.T. Barkema, J. Chem. Phys. (2003)