Brownian motion near cell membranes

Abdallah Daddi-Moussa-Ider, Achim Guckenberger and Stephan Gekle

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Biofluid Simulation and Modeling

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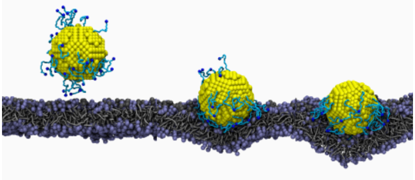
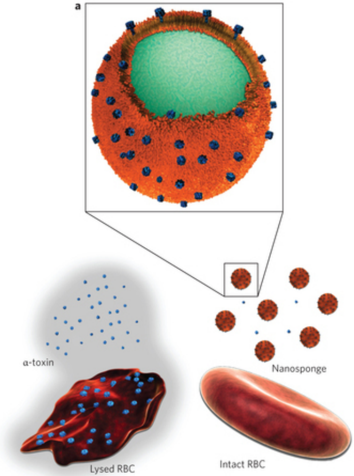
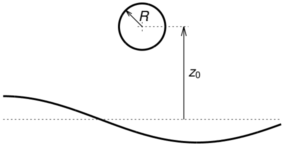


Li *et al.*, Biomaterials (2014)



Hu *et al.*, Nat Nano (2013)



Particle mobility

$$V_\alpha(\omega) = \mu_{\alpha\beta}(\boldsymbol{r}_0, \omega) F_\beta(\omega)$$

$$\mu_{\alpha\alpha}(\omega) = \mu_0 \exp\left(-R\sqrt{\frac{-i\rho\omega}{\eta}}\right) + \Delta\mu_{\alpha\alpha}(\omega)$$

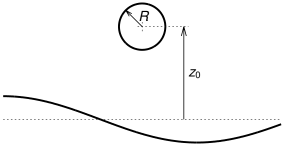
Equations of fluid motion

$$-\rho\frac{\partial \boldsymbol{v}}{\partial t} + \eta\nabla^2\boldsymbol{v} - \nabla p + \boldsymbol{F}\delta(\boldsymbol{r} - \boldsymbol{r}_0) = 0$$

$$\nabla \cdot \boldsymbol{v} = 0$$

The particle mobility serves as an input for diffusion.

How does the membrane affect the particle diffusional dynamics?



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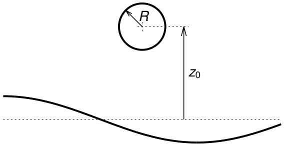

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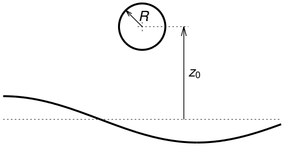

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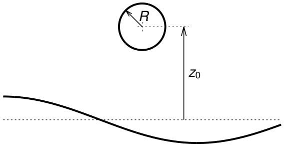

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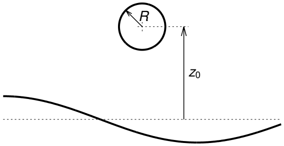

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Traction jumps

$$\text{Skalak} \quad \Delta f^{\beta} = -\frac{\kappa_{\mathrm{S}}}{3}\left(\Delta_{\parallel} u_{\beta} + (1+2C)e_{,\beta}\right), \quad \beta \in \{x, y\}$$

$$\text{Helfrich} \quad \Delta f^{z} = \kappa_{\mathrm{B}} \Delta_{\parallel}^{2} u_{z}$$

with $C = \kappa_{\mathrm{A}}/\kappa_{\mathrm{S}}$, $\Delta_{\parallel} = \partial_{,xx} + \partial_{,yy}$ and $e = u_{x,x} + u_{y,y}$ is the dilatation.

Velocity continuity

$$\boldsymbol{v}|_{z=0^+} - \boldsymbol{v}|_{z=0^-} = 0$$

No-slip condition

$$\boldsymbol{v} = \left.\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t}\right|_{z=0}$$

Resolution procedure

- Temporal Fourier transform $t \to \omega$
- Spatial two dimensional Fourier transform $(x, y) \to (q_x, q_y)$
- Passage to the new orthogonal system $(\boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z) \to (\boldsymbol{q}, \boldsymbol{t}, \boldsymbol{n})$

The fluid velocity field can then be found in Fourier space.

Felderhof, J. Chem. Phys. (2006), Bickel, PRE (2007)

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Mobility corrections

- Apply back spatial Fourier transform.
- Identify the velocity Green's functions from $v_\alpha = \mathcal{G}_{\alpha\beta} F_\beta$.
- Find the mobility correction in the point particle approximation.

$$\Delta\mu_{\alpha\beta}(\boldsymbol{r}_0, \omega) = \lim_{\boldsymbol{r}\to\boldsymbol{r}_0} \left(\mathcal{G}_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}_0) - \mathcal{G}^{(0)}_{\alpha\beta}(\boldsymbol{r} - \boldsymbol{r}_0) \right)$$

where $\mathcal{G}^{(0)}_{\alpha\beta}$ is the infinite space Green's function.

- The mobility correction tensor is diagonal such that $\Delta\mu_{xx} = \Delta\mu_{yy} = \Delta\mu_\parallel$ and $\Delta\mu_{zz} = \Delta\mu_\perp$.
- $\Delta\mu_\parallel$ and $\Delta\mu_\perp$ are conveniently expressed in terms of the following dimensionless numbers

$$\beta = \frac{12 z_0 \eta\omega}{\kappa_\mathrm{S} + \kappa_\mathrm{A}}, \quad \beta_\mathrm{B} = 2z_0 \left(\frac{4\eta\omega}{\kappa_\mathrm{B}}\right)^{1/3}, \quad \sigma = z_0 \left(\frac{\rho\omega}{\eta}\right)^{1/2}$$

Analytical expression are possible for the steady Stokes equations.

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Brownian dynamics

The particle dynamics is governed by the generalized Langevin equation

$$m\frac{\mathrm{d}v_\alpha}{\mathrm{d}t} = -\int_{-\infty}^{t} \zeta_\alpha(t-t')v_\alpha(t')\mathrm{d}t' + F(t)\,, \quad \alpha \in \{\parallel, \perp\}$$

The particle mean squared displacement (MSD) is computed as

$$\langle x_\alpha(t)^2\rangle = 2\int_0^t (t-s)\phi_{v,\alpha}(s)\mathrm{d}s$$

Kubo, Toda and Hashitsume, Stat. Phys. II (1985)

$$\text{Excess MSD:} \quad \Delta_\alpha(t) := 1 - \frac{\langle x_\alpha(t)^2\rangle}{2D_0 t} = 1 - \frac{D(t)}{D_0}, \quad D_0 = k_\mathrm{B} T\mu_0$$

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Boundary integral methods

A completed double layer boundary integral equation method is used.

Zhao, Shaqfeh and Narsimhan, Phys. of Fluids (2012)

The traction jumps are computed according to the Skalak and Helfrich models.

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The particle and the membrane velocities are found after solving a linear system of equations.

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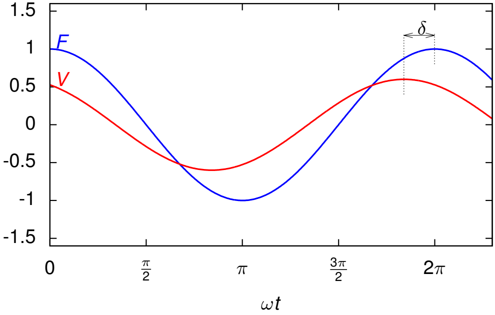
Mobility simulations

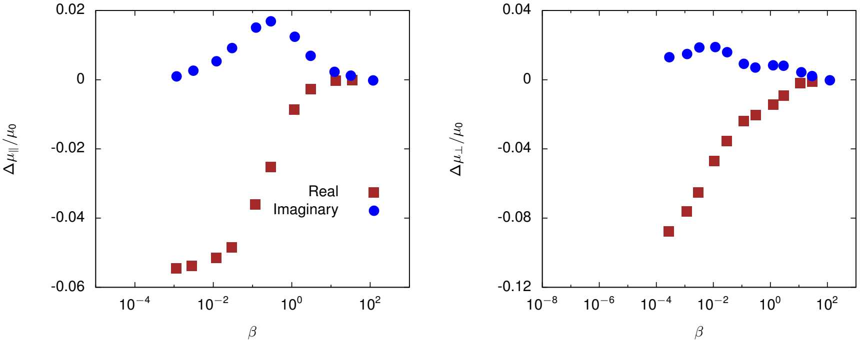
- An oscillating force $\boldsymbol{F}_0 e^{i\omega t}$ is applied on the particle.
- The recorded velocity is fitted as $\boldsymbol{V}_0 e^{i(\omega t+\delta)}$.
- The frequency dependent mobility is evaluated from

$$\mu(\omega) = \frac{V_0}{F_0} e^{i\delta}$$



Analytics v.s. numerics

A series of simulations are performed over a range of frequencies.
Here $R/z_0 = 0.1$ and $\kappa_B/R^2\kappa_S = 0.5$.



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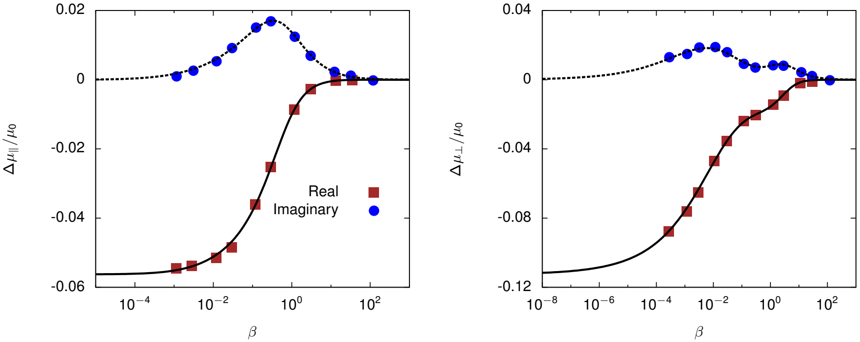

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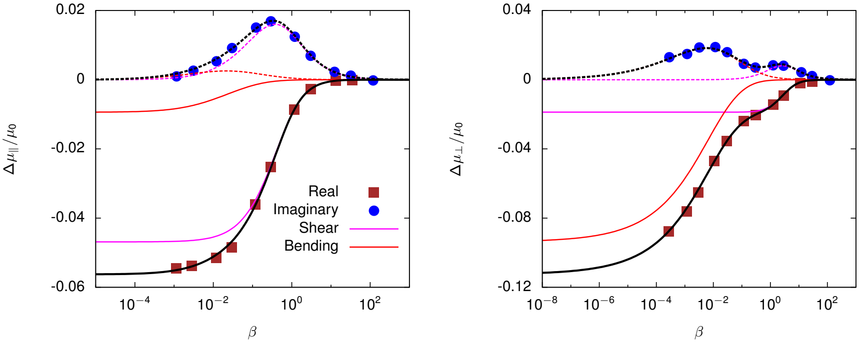

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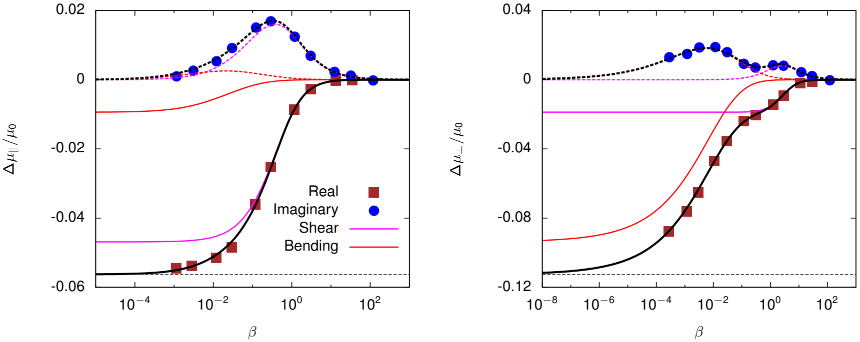

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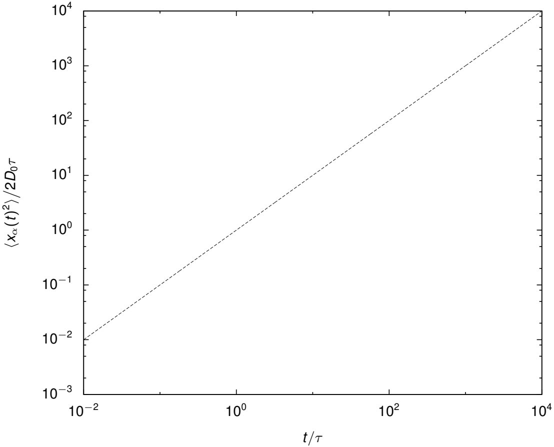

For typical cell parameters $\tau \sim 0.4$ms.

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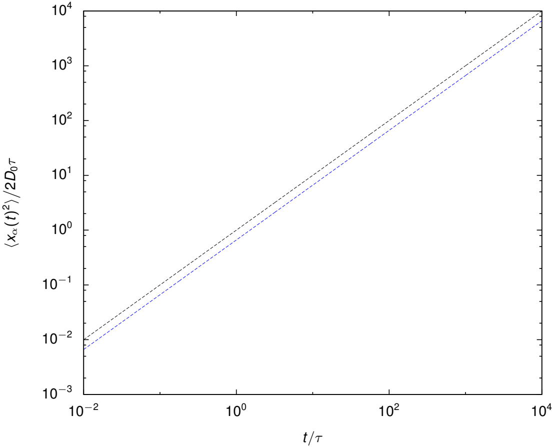

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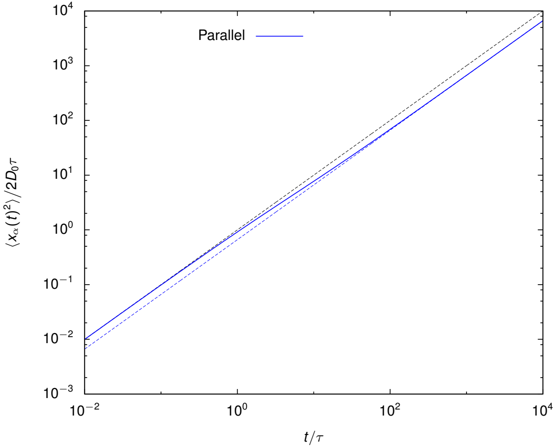

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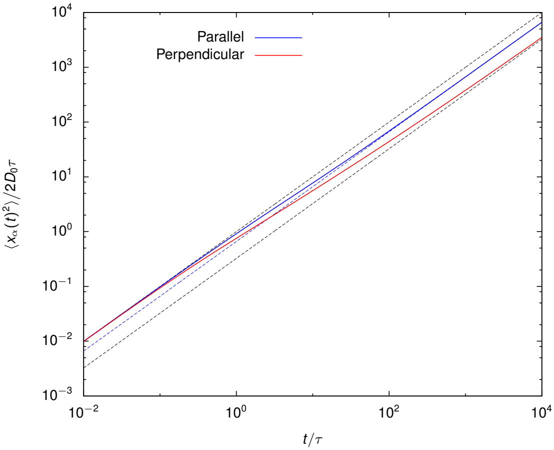

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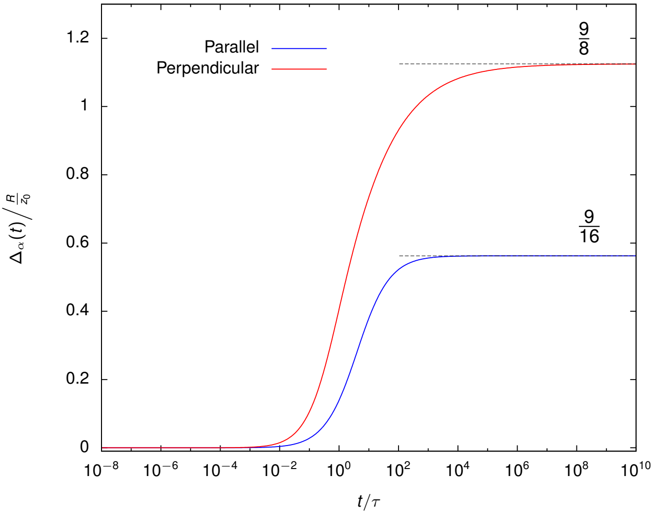
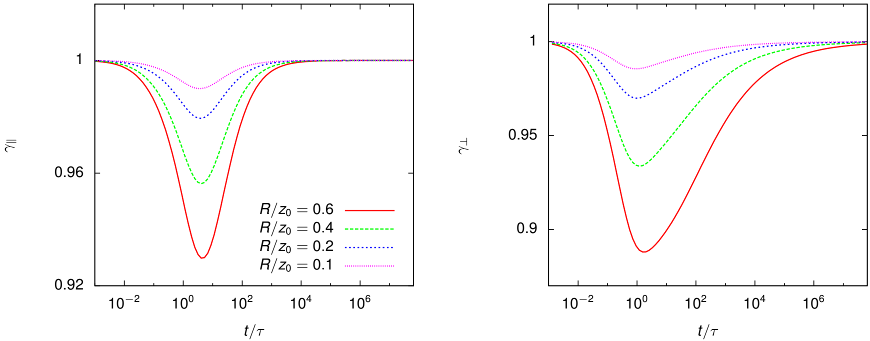

Parallel
Perpendicular
9/8
9/16
1.2
1
0.8
0.6
0.4
0.2
0
10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} 10^{2} 10^{4} 10^{6} 10^{8} 10^{10}
t/τ
$\Delta_\alpha(t) / \frac{R}{z_0}$

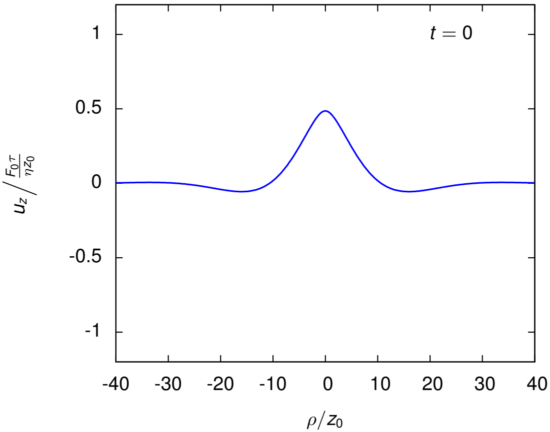
Scaling exponent

$$\gamma_\alpha(t) := \frac{\mathrm{d}\ln\langle x_\alpha(t)^2\rangle}{\mathrm{d}\ln t} = 1 - \frac{t\Delta'(t)}{1-\Delta(t)}$$



Membrane vertical displacement (Perpendicular motion)

- The motion of the interface can be investigated.
- Here the force is applied perpendicular to the membrane.



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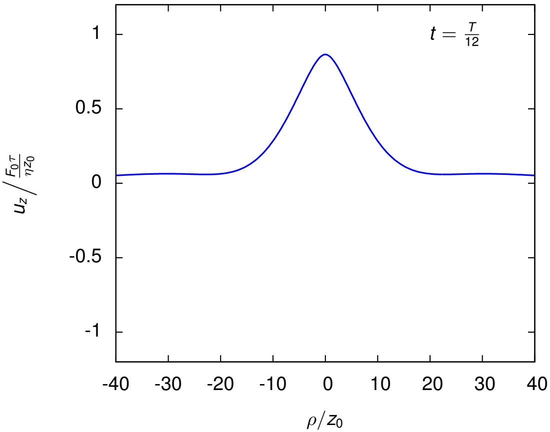

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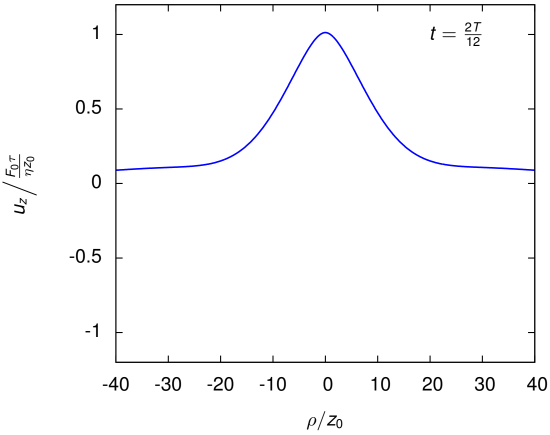

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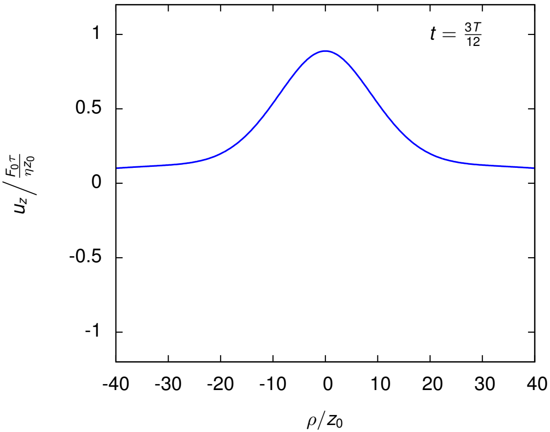

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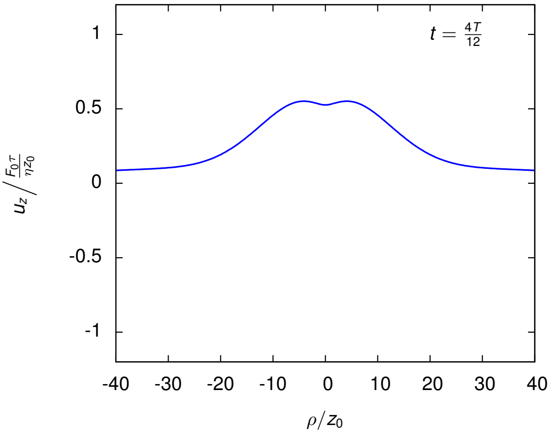

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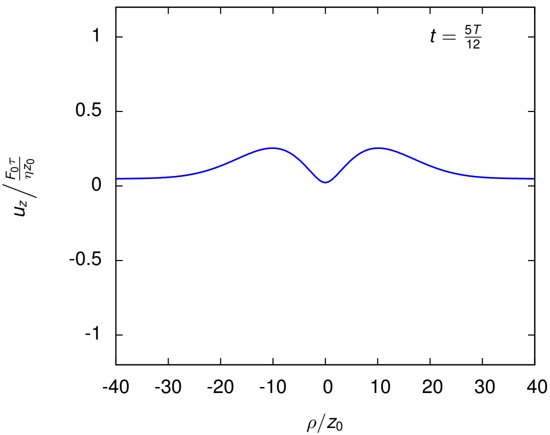

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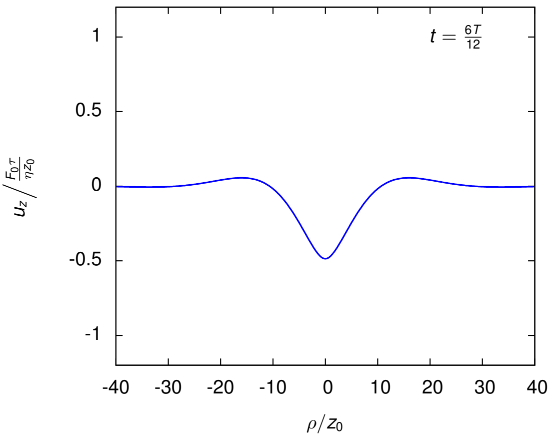

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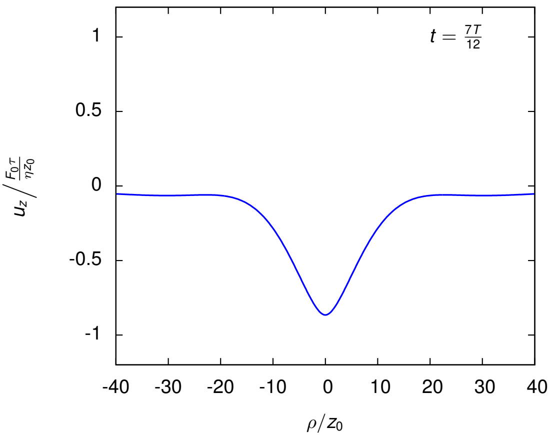

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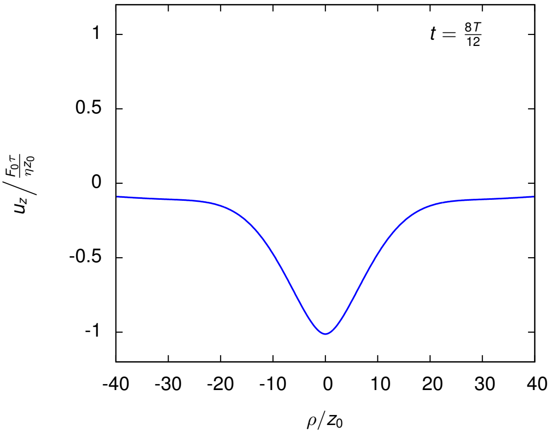

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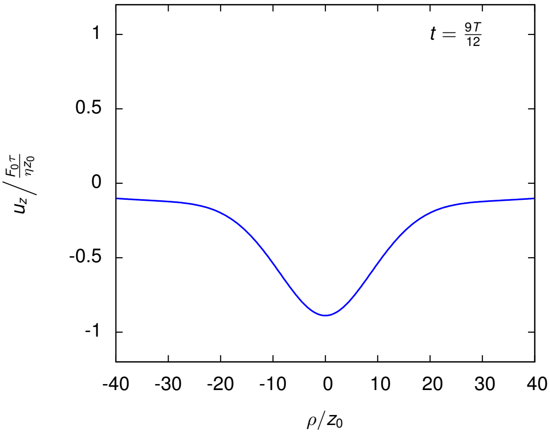

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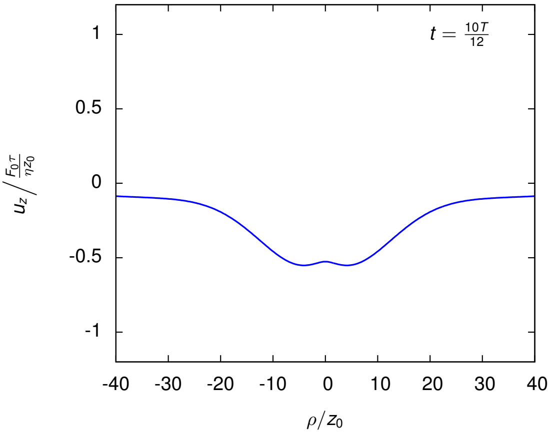

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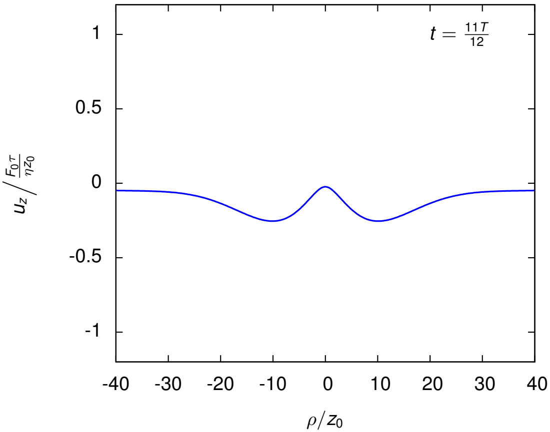

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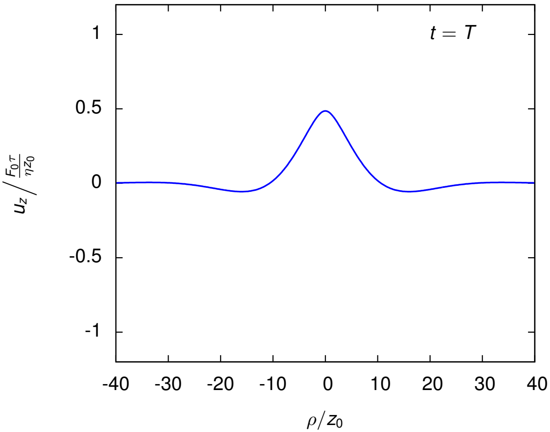

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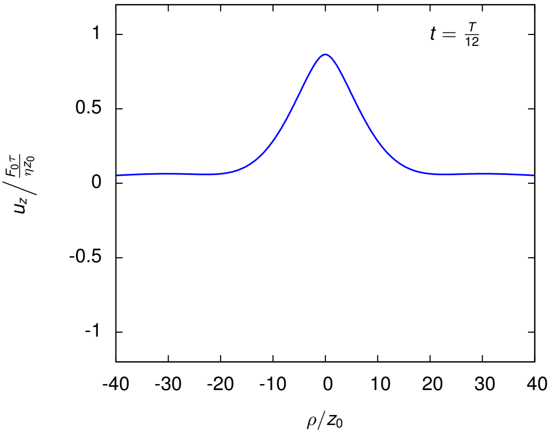

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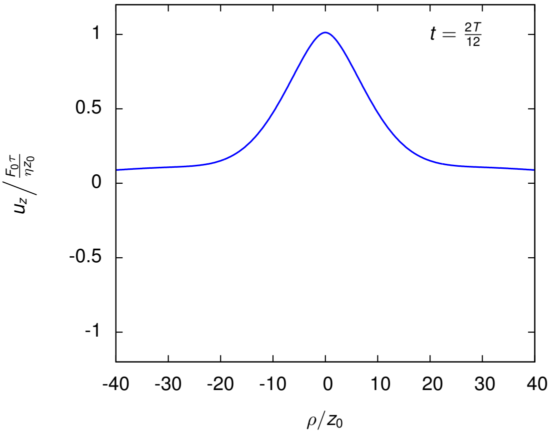

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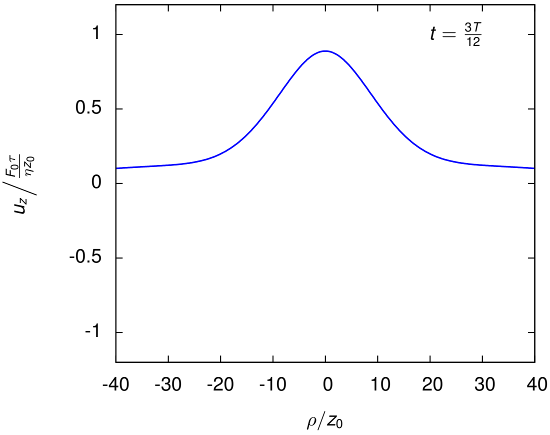

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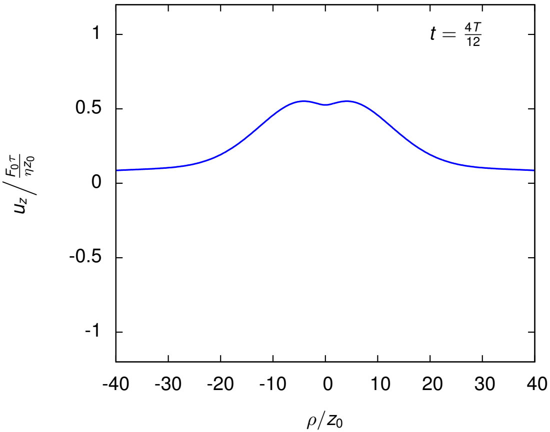

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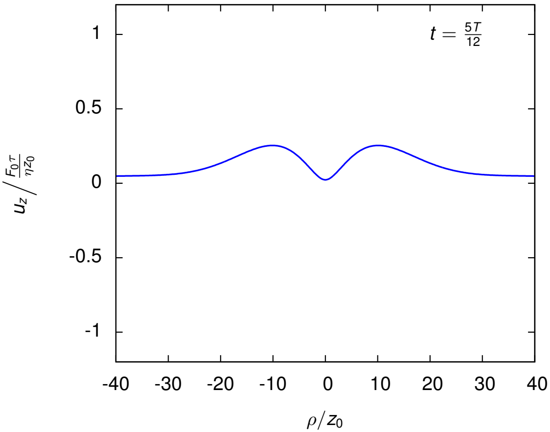

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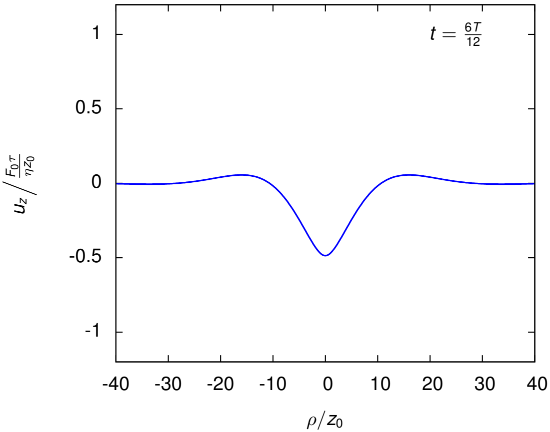

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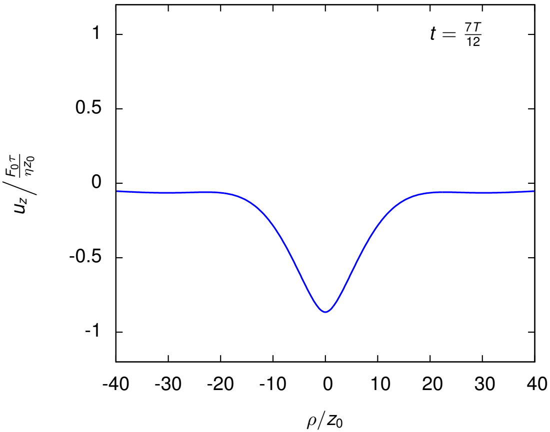

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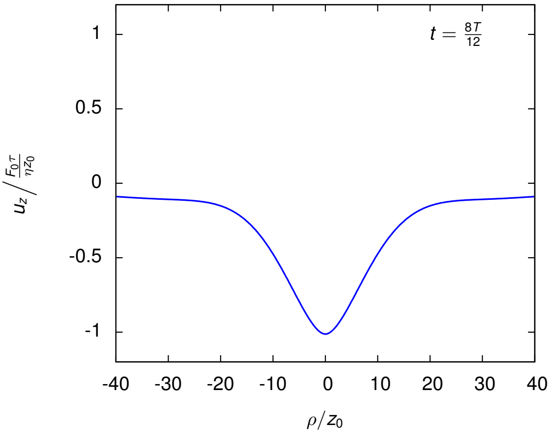

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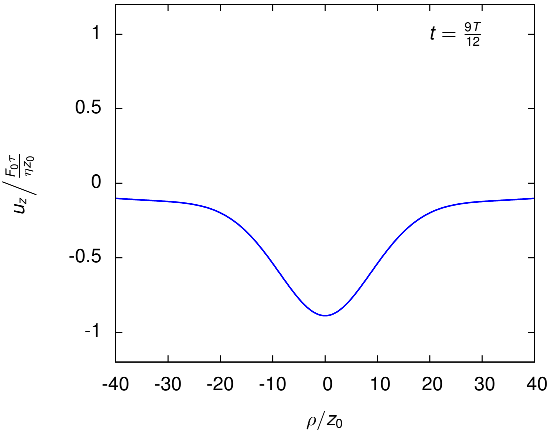

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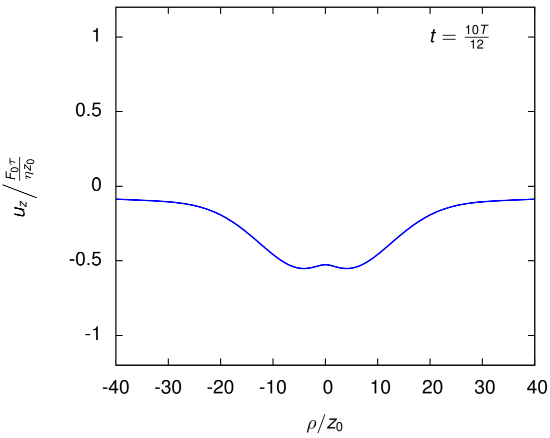

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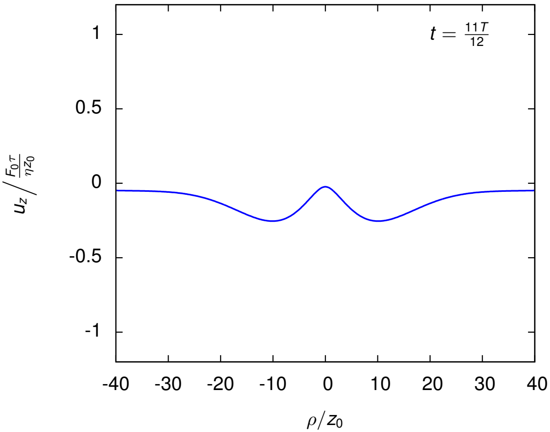

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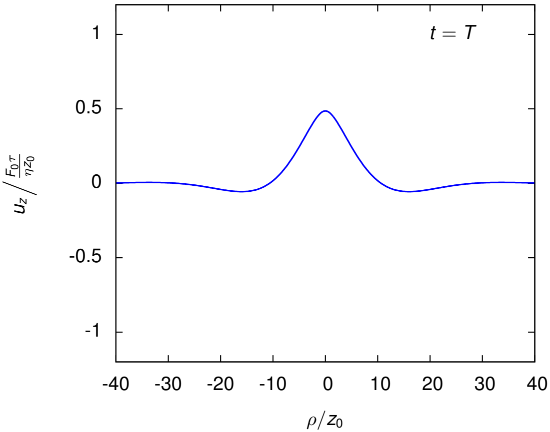

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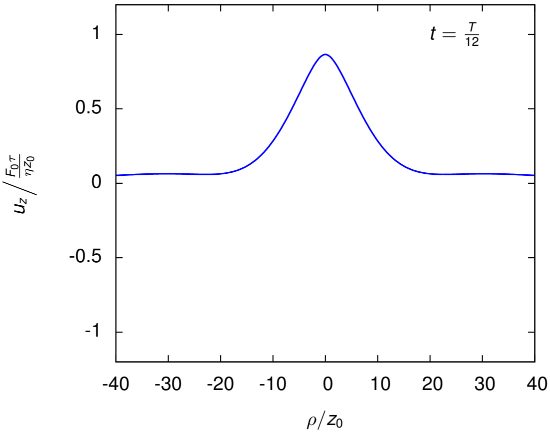

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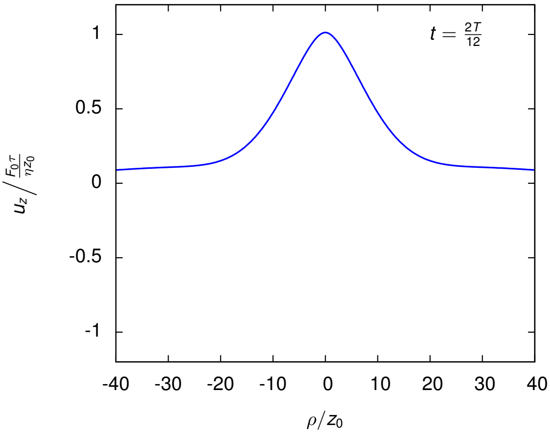

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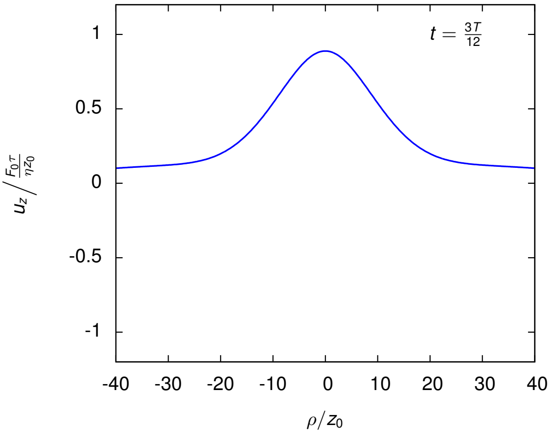

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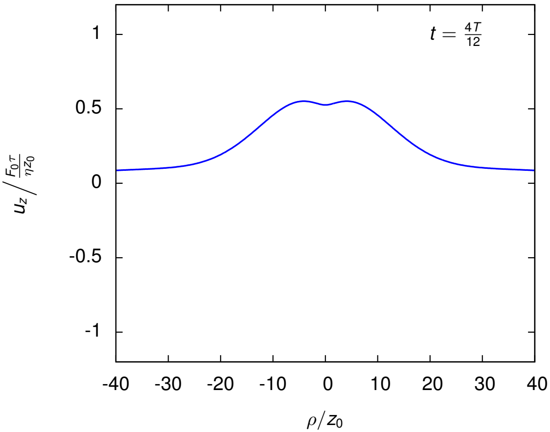

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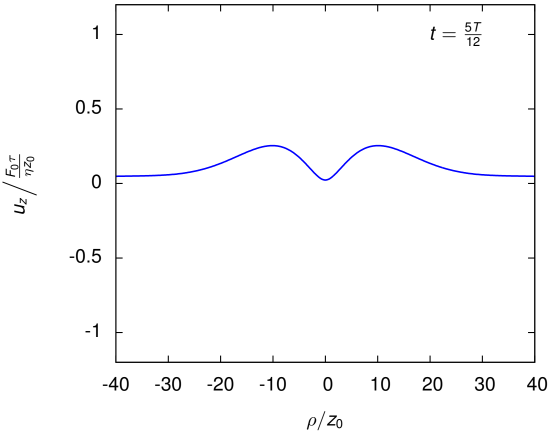

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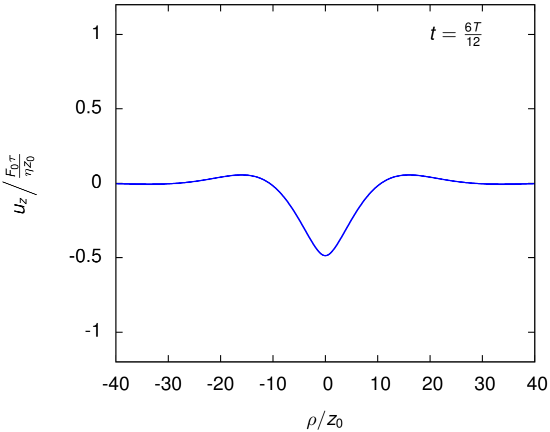

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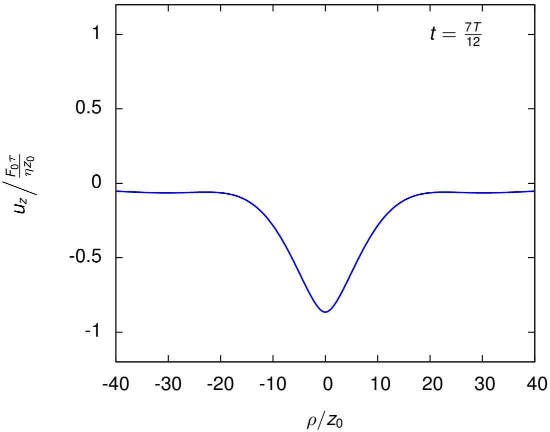

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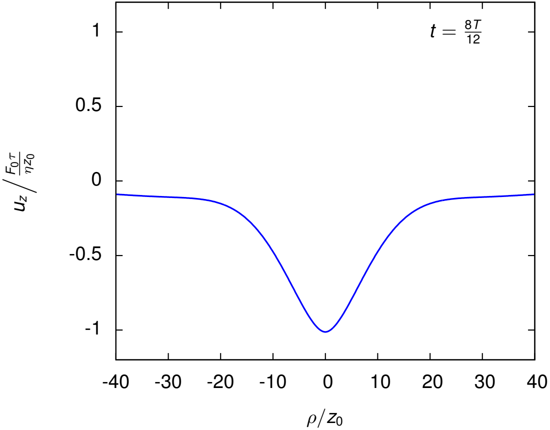

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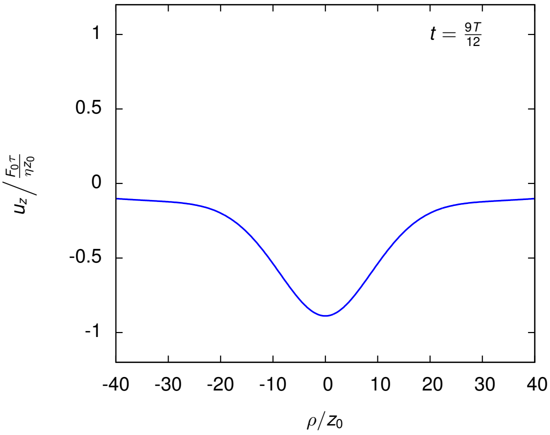

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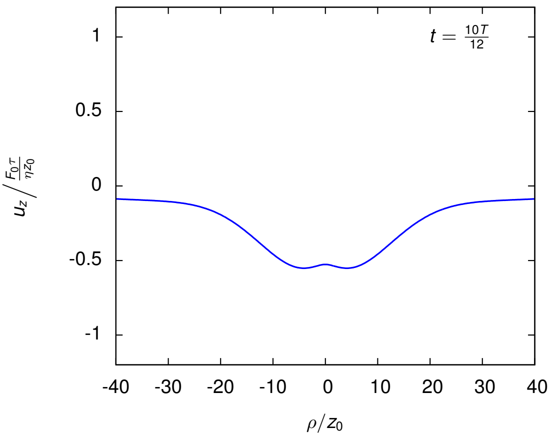

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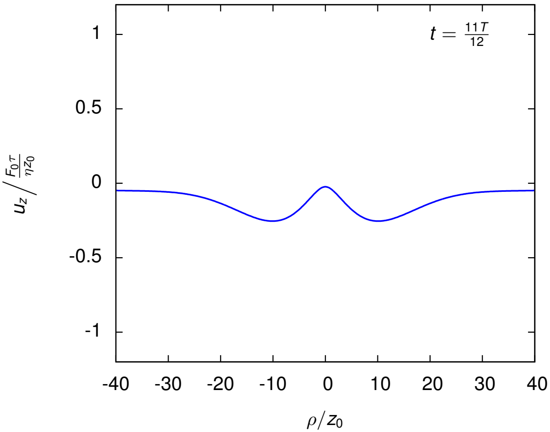

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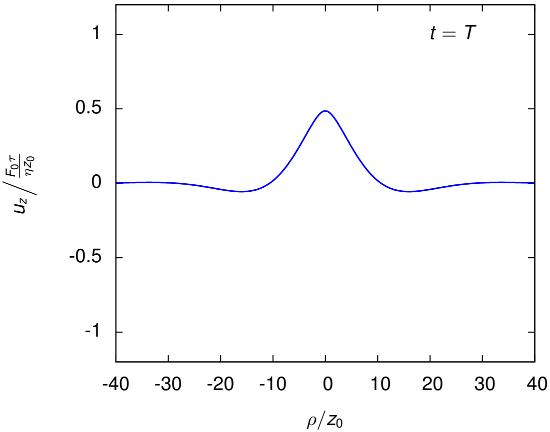

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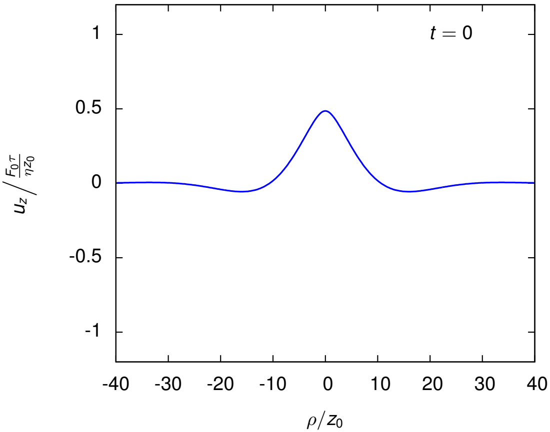

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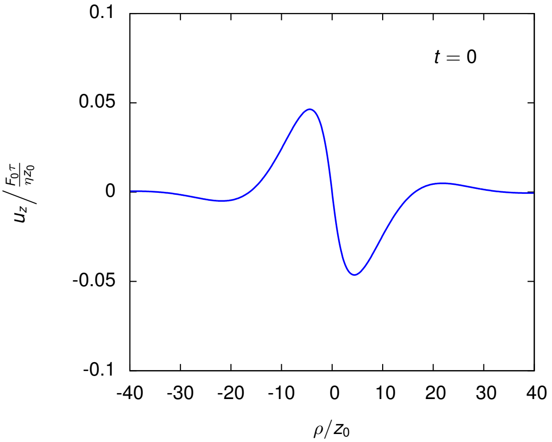

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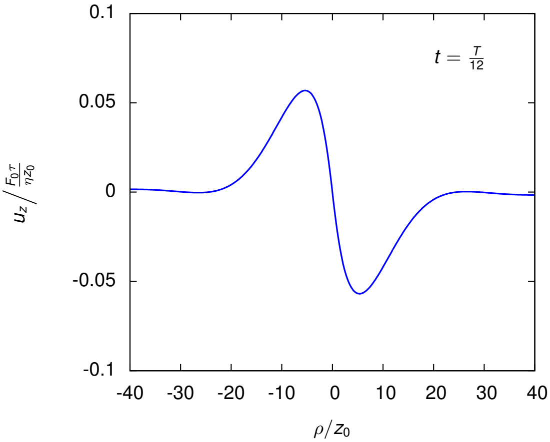

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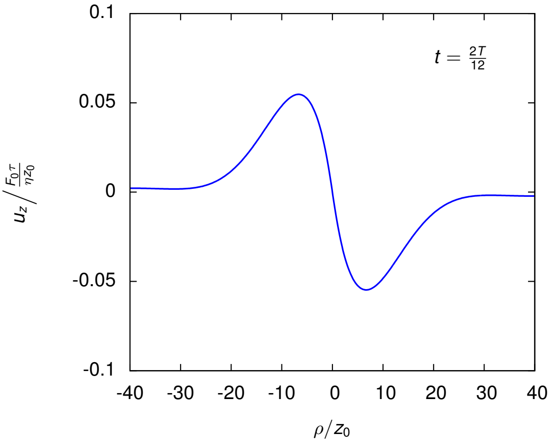

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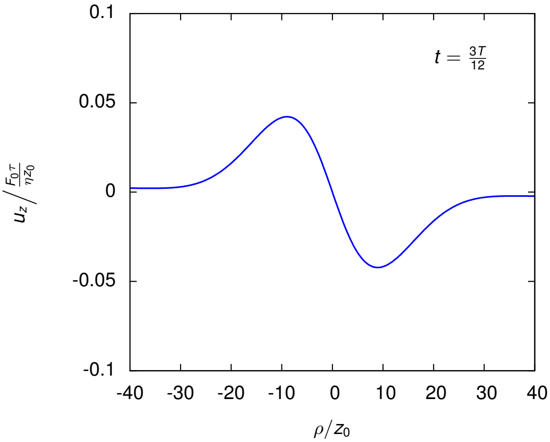

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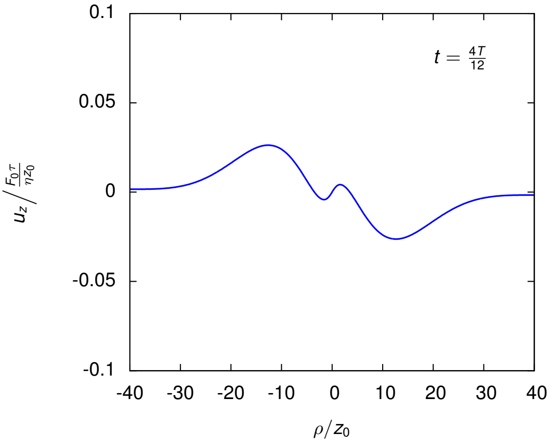

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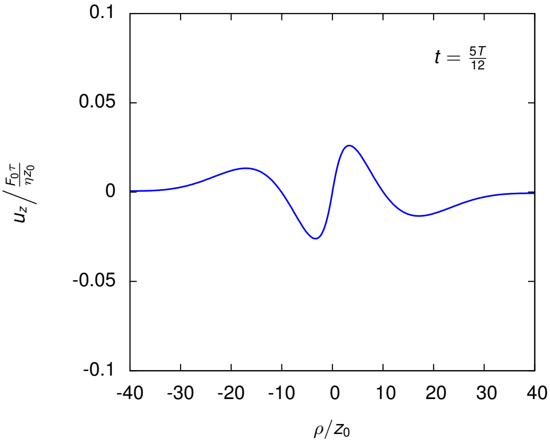

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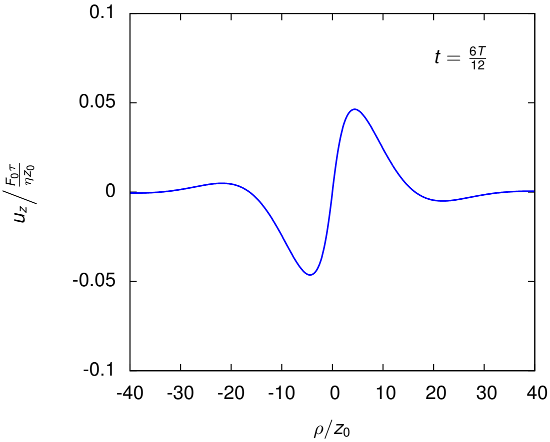

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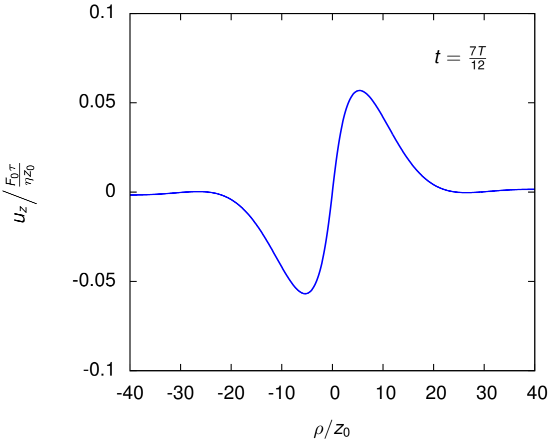

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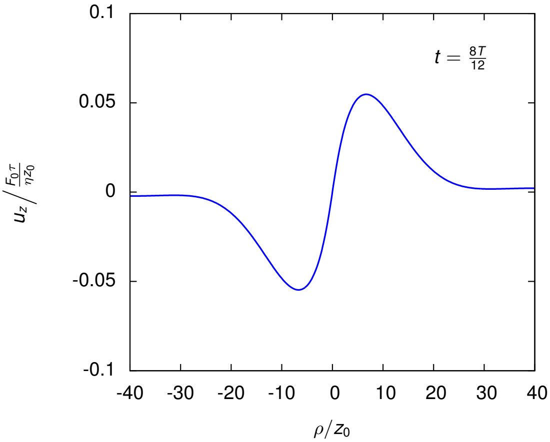

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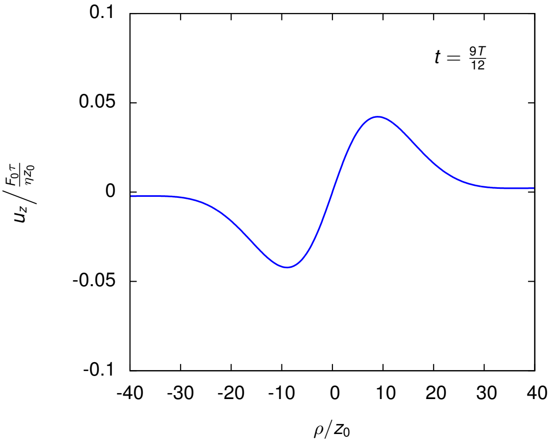

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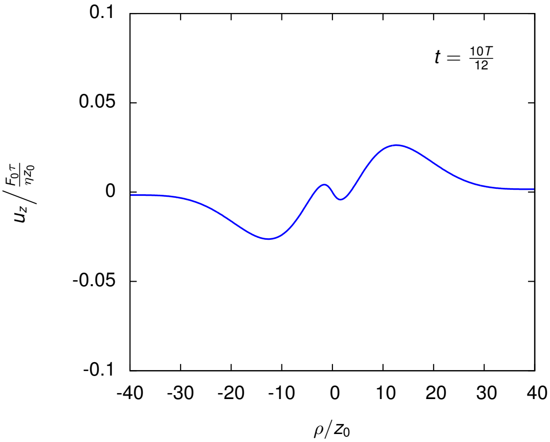

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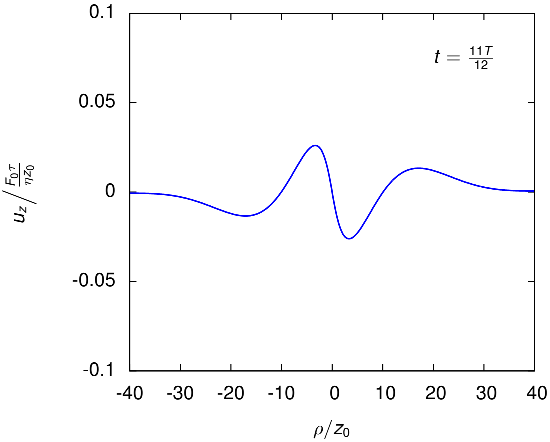

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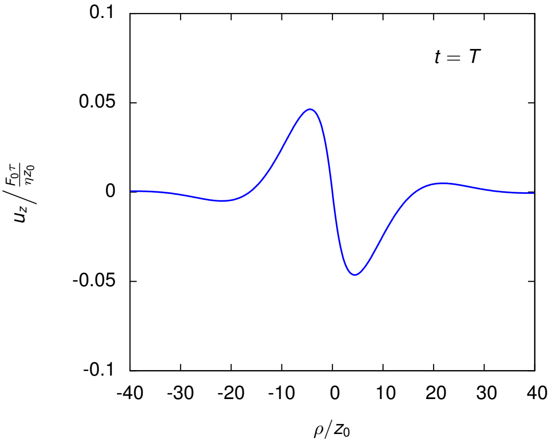

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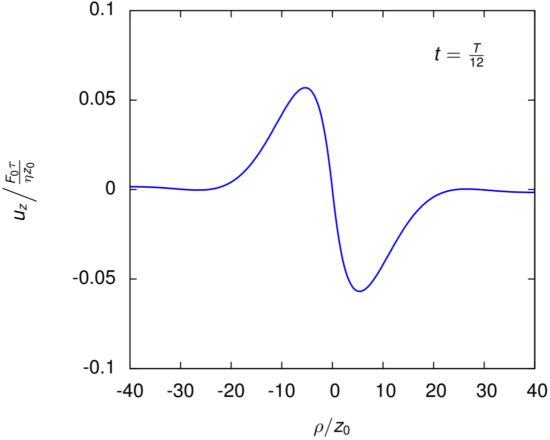

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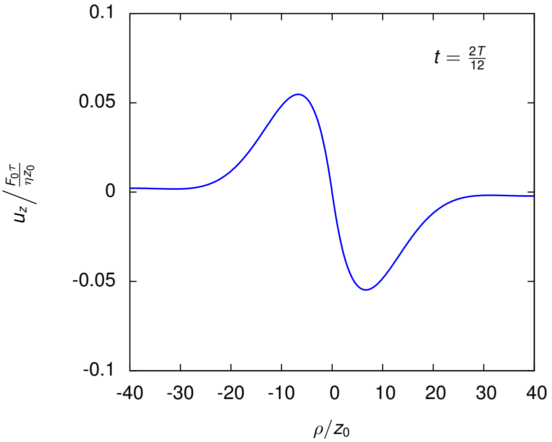

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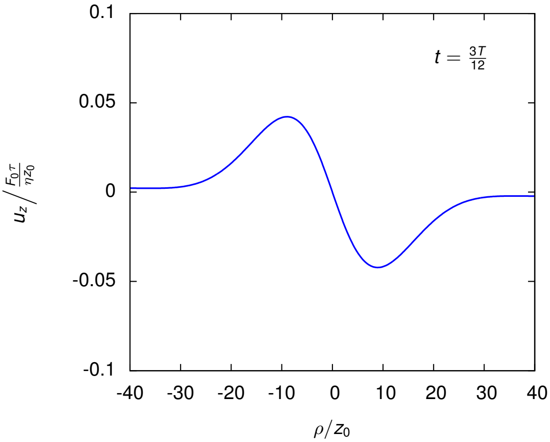

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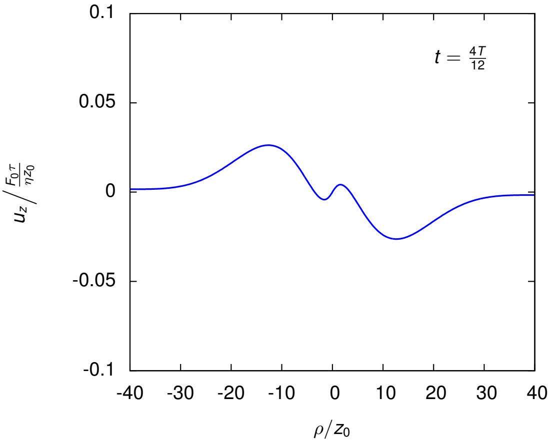

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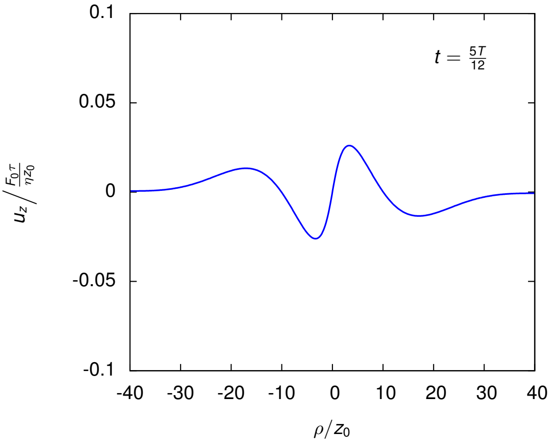

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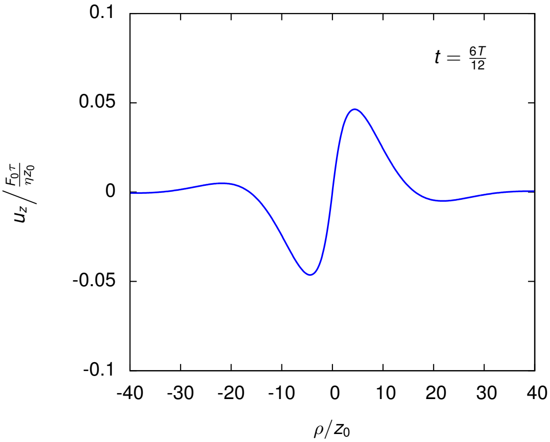

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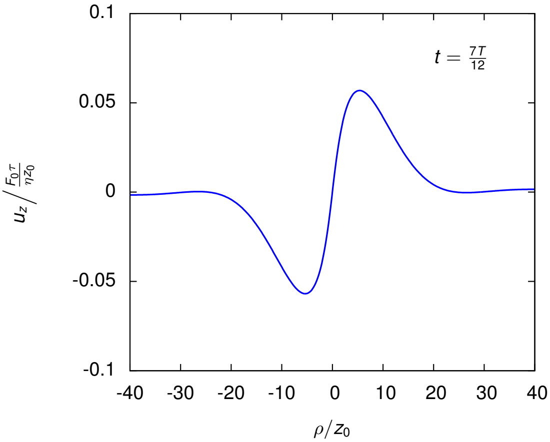

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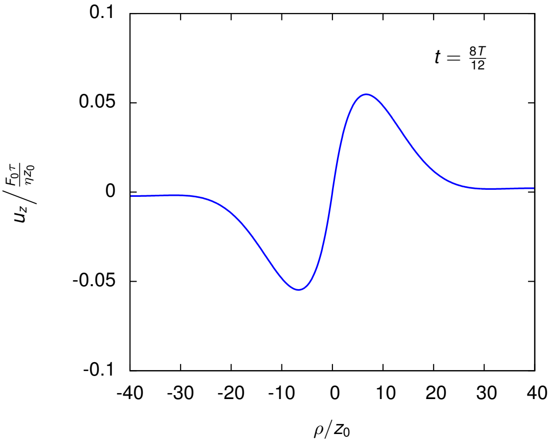

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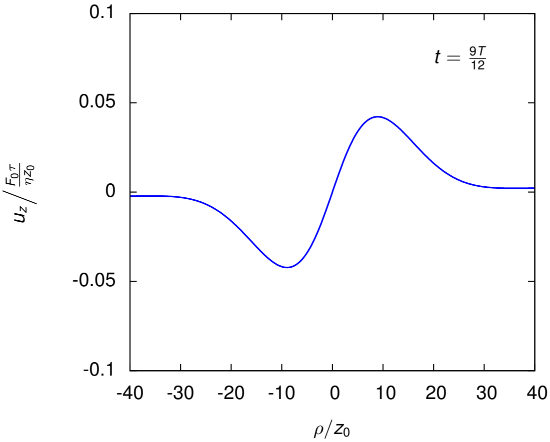

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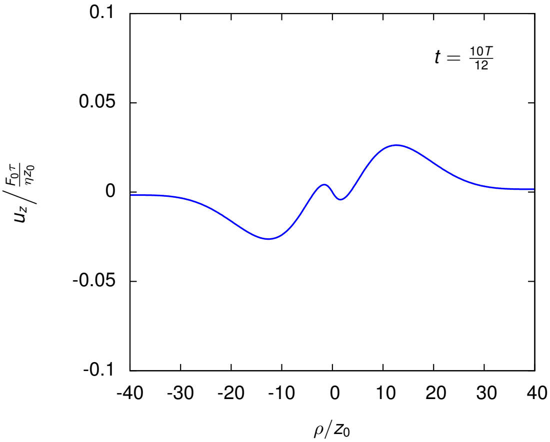

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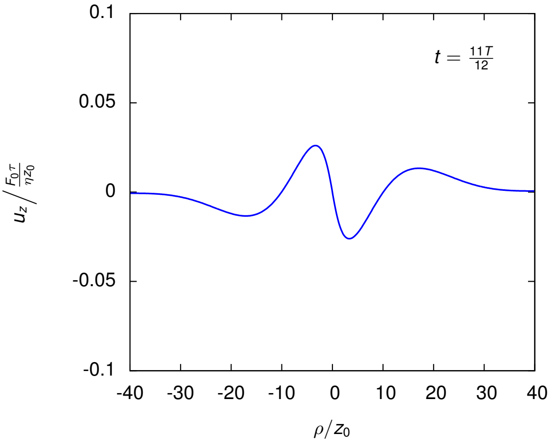

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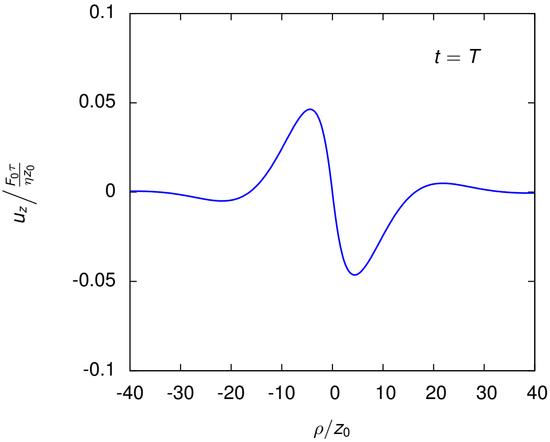

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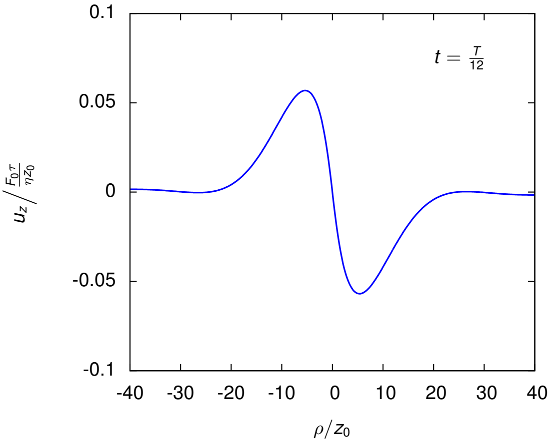

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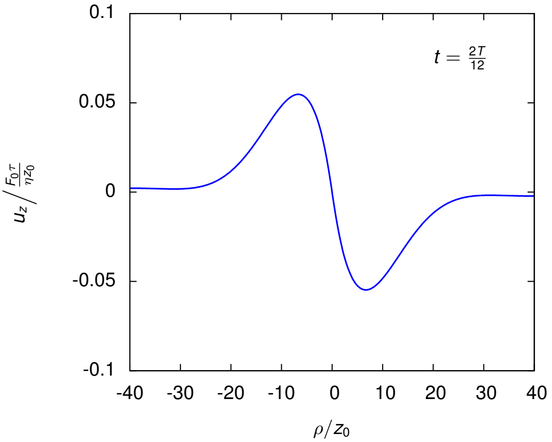

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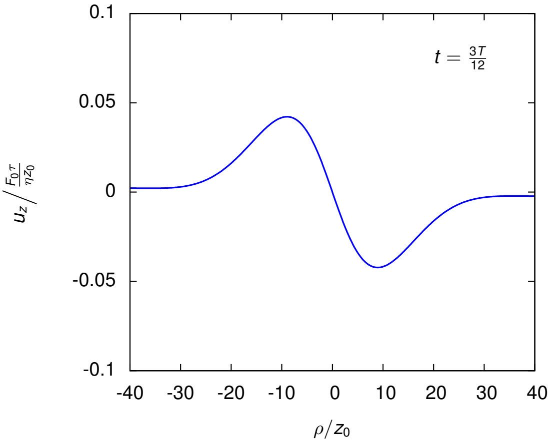

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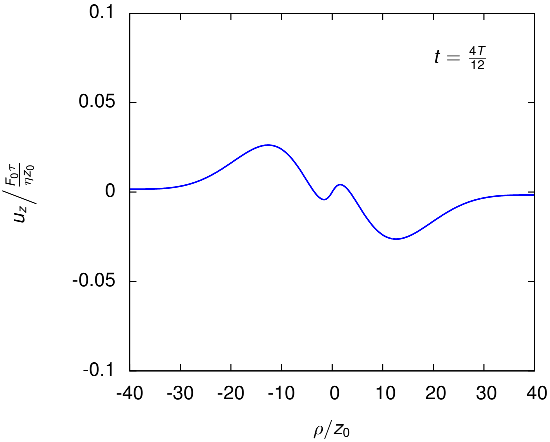

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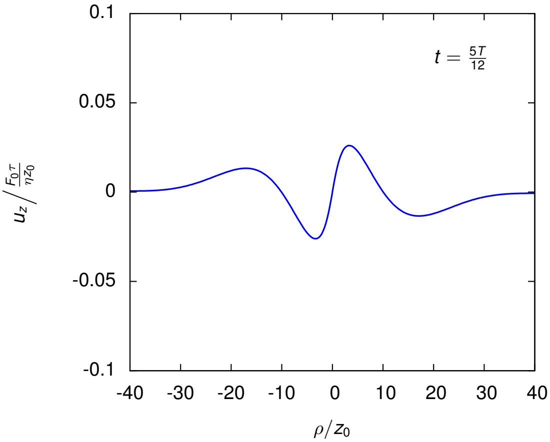

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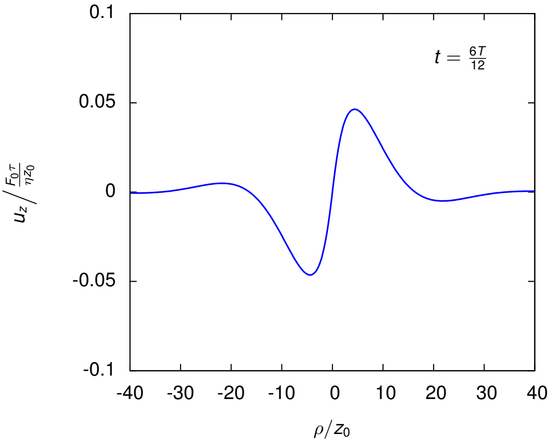

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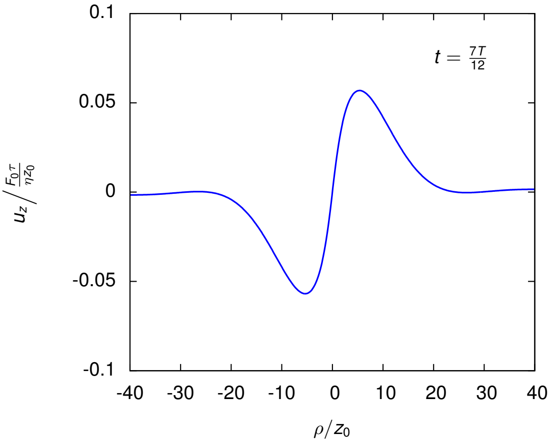

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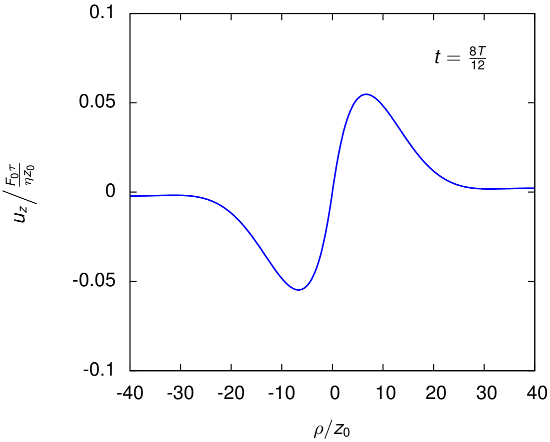

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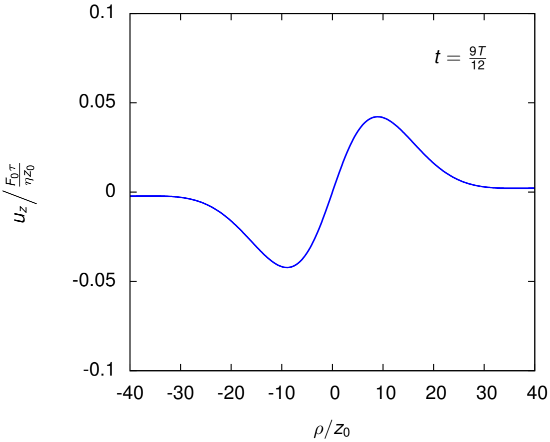

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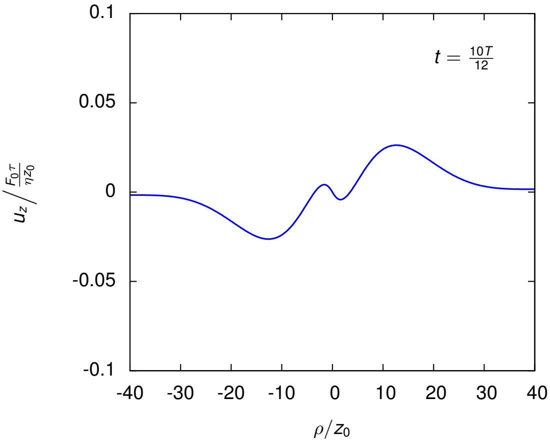

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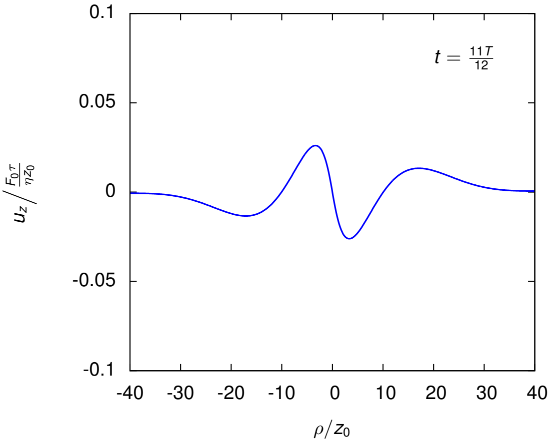

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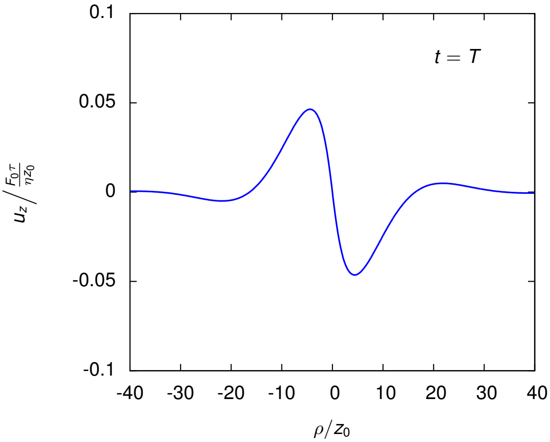

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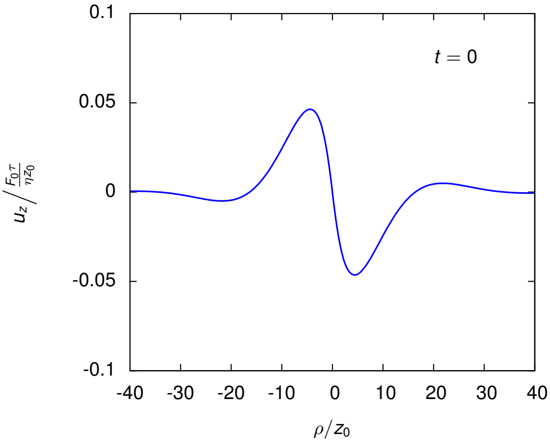

To summarize

- Induced long-lived anomalous diffusion on particles near elastic membranes.
- The long-time diffusion coefficient is identical to that near a hard wall.
- Perpendicular diffusion is significantly slower than parallel diffusion.
- Shear and area dilatation are dominant in the parallel direction whereas bending is dominant in the perpendicular direction.

ADMI, Guckenberger and Gekle Accepted Phys. Rev. E (2016)

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Boundary integral methods

A completed double layer boundary integral equation method is used.

$$v_j(\boldsymbol{x}) = H_j(\boldsymbol{x})\,, \quad \boldsymbol{x} \in S_{\mathrm{m}}$$

$$\frac{1}{2}\phi_j(\boldsymbol{x}) + \sum_{i=1}^{6} \varphi_j^{(i)}(\boldsymbol{x})\langle \varphi^{(i)}, \boldsymbol{\phi}\rangle = H_j(\boldsymbol{x})\,, \quad \boldsymbol{x} \in S_{\mathrm{p}}$$

where

$$H_j(\boldsymbol{x}) \equiv -\frac{1}{8\pi\eta}(N_{\mathrm{m}}\Delta \boldsymbol{f}_j)(\boldsymbol{x}) - \frac{1}{8\pi}(K_{\mathrm{p}}\boldsymbol{\phi})_j(\boldsymbol{x}) + \frac{1}{8\pi\eta}G_{jk}(\boldsymbol{x}, \boldsymbol{x}_{\mathrm{c}})F_k$$

Zhao, Shaqfeh and Narsimhan, Phys. of Fluids (2012)