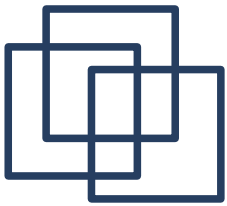


mgr inż. Marcin Kędzierski

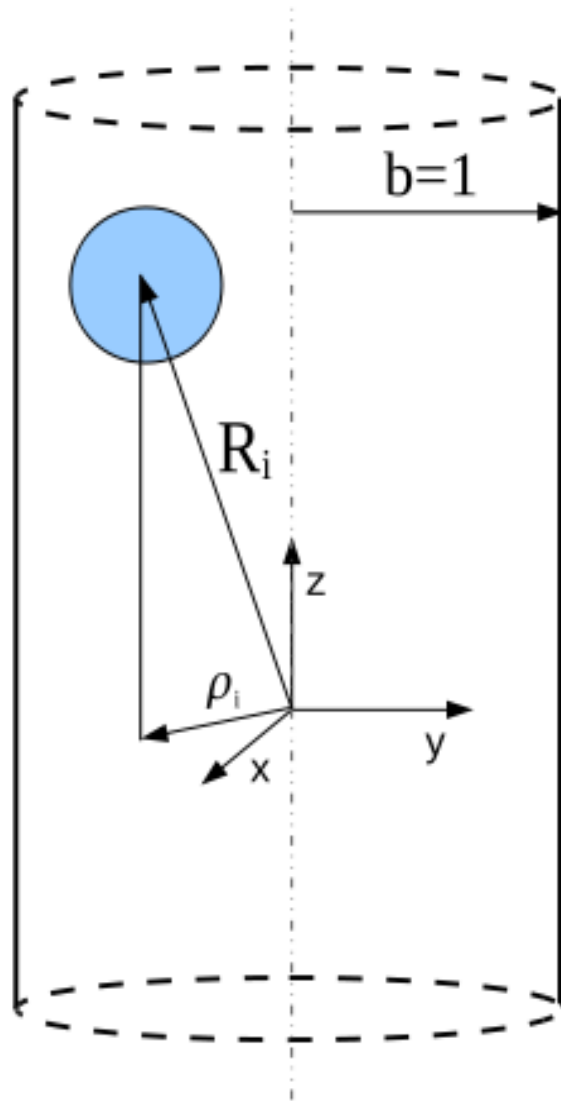
Oddziaływania
hydrodynamiczne w
cylindrycznym mikrokanale



Zakład Mechaniki i Fizyki Płynów



Układ i założenia

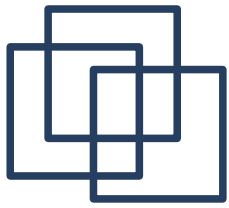


1. koloid złożony z cząstek
- недеформовalnych
- сферических
- неброуновских
zanurzony w nieścislwym płynie

2. $Re \ll 1$

$$\eta \nabla^2 \mathbf{v} - \nabla p = -\mathbf{f}(\mathbf{r})$$

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



Założenie 3.

skala
czasowa
związana z
dynamiką
cząstek

$$\longrightarrow t \gg \tau_{vis} \approx \tau_{vel}$$

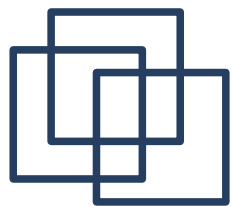
$$\tau_{vis} = \frac{a^2 \rho}{\eta}$$

czas lepkiej
relaksacji zaburzeń
prędkości cieczy

$$\tau_{vel} = \frac{m}{\xi} = \frac{2a^2 \rho_{par}}{9\eta}$$

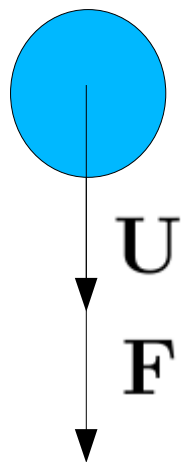
$$\xi = 6\pi\eta a$$

czas relaksacji
prędkości cząstki w
płynie



Oddziaływania hydrodynamiczne

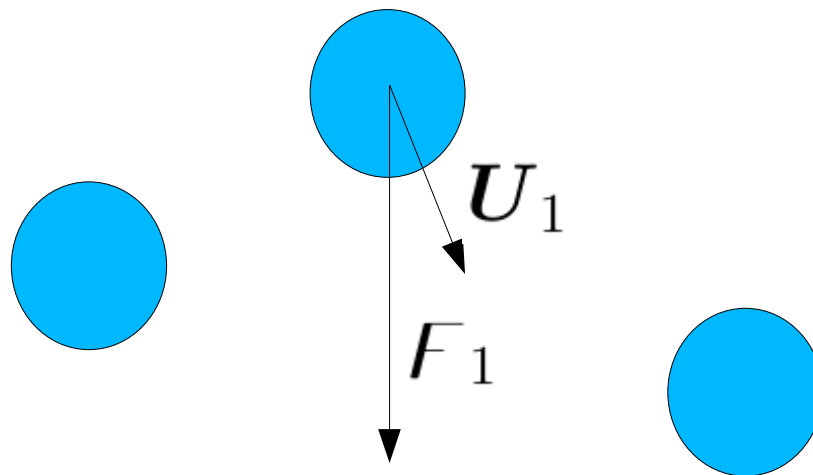
1 cząstka



$$\mathbf{F} = \xi \mathbf{U}$$

$$\xi = 6\pi\eta a$$

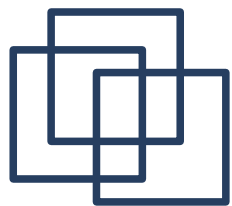
układ N-cząstkowy



$$F = \xi \cdot U$$

$$F = (F_1, \dots, F_N)$$

$$U = (U_1, \dots, U_N)$$



Równanie całkowe

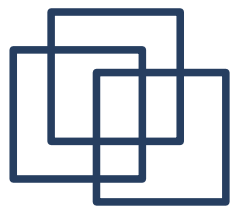
$$\eta \nabla^2 \mathbf{v} - \nabla p = -\mathbf{f}(\mathbf{r})$$

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

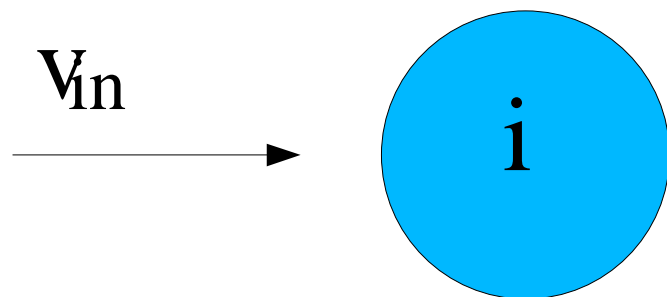


$$\mathbf{v}_i^{rb}(\mathbf{r}) - \mathbf{v}_\infty(\mathbf{r}) = \int \mathbf{Z}_i^{-1}(\mathbf{r} - \mathbf{R}_i, \mathbf{r}' - \mathbf{R}_i) \cdot \mathbf{F}_i(\mathbf{r}') d\mathbf{r}'$$

$$+ \sum_{j=1}^N \int [1 - \delta_{ij} \mathbf{T}_0(\mathbf{r} - \mathbf{r}') + \mathbf{T}_b(\mathbf{r}, \mathbf{r}')] \cdot \mathbf{F}_j(\mathbf{r}') d\mathbf{r}', \mathbf{r} \in S_i$$

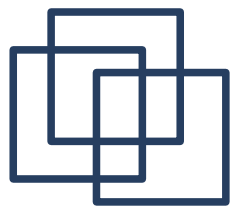


Operator



$$\mathbf{F}_i(\mathbf{r}) = - \int \mathbf{Z}_i(\mathbf{r} - \mathbf{R}_i, \mathbf{r}' - \mathbf{R}_i) \cdot (\mathbf{v}_i^{in}(\mathbf{r}') - \mathbf{v}_i^{rb}(\mathbf{r}')) d\mathbf{r}'$$

$$\mathbf{T}_0(\mathbf{r}) = \frac{1}{8\pi\eta r} \left(\mathbf{1} + \frac{\mathbf{r}\mathbf{r}}{r^2} \right)$$



Projekcja

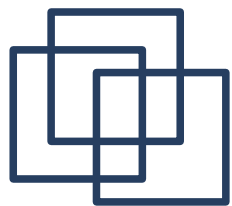
$$\mathbf{v}_i^{rb}(\mathbf{r}) - \mathbf{v}_\infty(\mathbf{r}) = \int \mathbf{Z}_i^{-1}(\mathbf{r} - \mathbf{R}_i, \mathbf{r}' - \mathbf{R}_i) \cdot \mathbf{F}_i(\mathbf{r}') d\mathbf{r}'$$

$$+ \sum_{j=1}^N \int [1 - \delta_{ij} \mathbf{T}_0(\mathbf{r} - \mathbf{r}') + \mathbf{T}_b(\mathbf{r}, \mathbf{r}')] \cdot \mathbf{F}_j(\mathbf{r}') d\mathbf{r}', \mathbf{r} \in S_i$$

Projekcja na bazę
sferyczną



Równanie algebraiczne



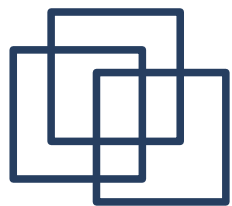
Baza sferyczna

kobaza

baza regularna

baza singularna

$$\langle \mathbf{w}_{lm\sigma}^{\pm}(\mathbf{r}) \delta_a | \mathbf{v}_{l_1 m_1 \sigma_1}^{\pm}(\mathbf{r}) \rangle = \delta_{ll_1} \delta_{mm_1} \delta_{\sigma\sigma_1}$$



Metoda multipolowa

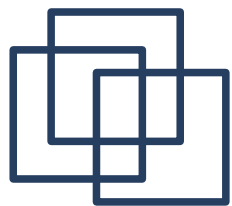
$$c_i(lm\sigma) = \sum_{j=1}^N \sum_{l'=1}^{\infty} \sum_{m'=-l'}^{l'} \sum_{\sigma'=0}^2 M_{ij}(lm\sigma, l'm'\sigma') f_j(l'm'\sigma')$$

$$f_j(lm\sigma) = \int \mathbf{v}_{lm\sigma}^{+*}(\mathbf{r}' - \mathbf{R}_j) \cdot \mathbf{F}_j(\mathbf{r}') d\mathbf{r}'$$

multipole siły

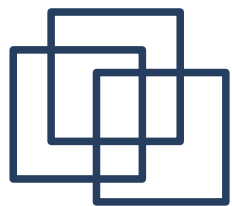
$$c_i(lm\sigma) = \int \frac{1}{a} \delta(|\mathbf{r}' - \mathbf{R}_j| - a) w_{lm\sigma}^{+*}(\mathbf{r}' - \mathbf{R}_j) \cdot (\mathbf{v}_i^{rb}(\mathbf{r}') - \mathbf{v}_{\infty}(\mathbf{r}')) d\mathbf{r}'$$

multipole prędkości



Metoda multipolowa

$$\begin{aligned} M_{ij}(lm\sigma, l'm'\sigma') &= \delta_{ij} Z_i^{-1}(lm\sigma, l'm'\sigma') \\ &+ (1 - \delta_{ij}) T_{ij}^0(lm\sigma, l'm'\sigma') \\ &+ T_{ij}^b(lm\sigma, l'm'\sigma'), \end{aligned}$$



Metoda multipolowa

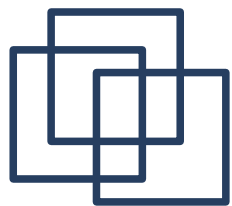
$$T_{ij}^0(lm\sigma, l'm'\sigma') = \frac{1}{\eta} \frac{n_{lm}}{n_{l'm'}} S^{+-}(\mathbf{R}_i - \mathbf{R}_j; lm\sigma, l'm'\sigma')$$

(Felderhof, Jones 1989)

$Z_i^{-1}(lm\sigma, l'm'\sigma')$

- twarde sfery
- krople
- sfery pokryte surfaktantem
- ...

CEL: $T_{ij}^b(lm\sigma, l'm'\sigma')$

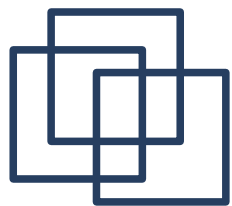


Metoda multipolowa

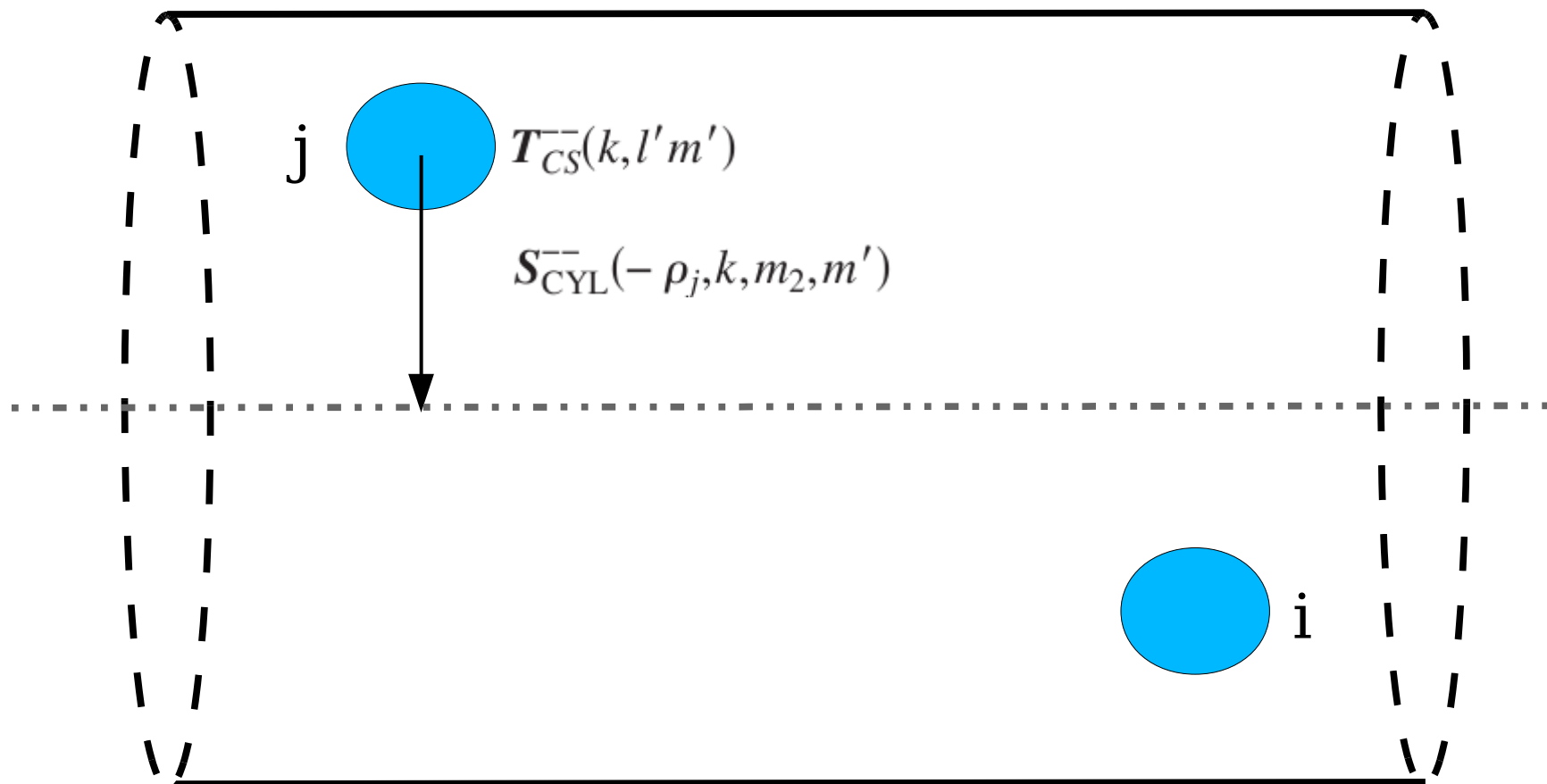
$$\mathbf{T}_{ij}^b(lm, l' m') = -\frac{1}{\eta} \sum_{m_2=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathbf{g}_{lm, l' m'}(m_2, k; \boldsymbol{\rho}_i, \boldsymbol{\rho}_j) e^{ik(z_i - z_j)} dk$$

$$\mathbf{g}_{lm, l' m'}(m_2, k; \boldsymbol{\rho}_i, \boldsymbol{\rho}_j)$$

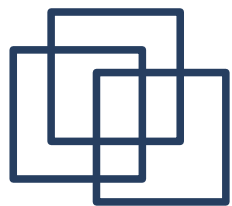
$$\begin{aligned} &= \mathbf{T}_{SC}^{++}(lm, k) \cdot \mathbf{S}_{CYL}^{++}(\boldsymbol{\rho}_i, k, m, m_2) \cdot \mathbf{Z}_C(k, m_2) \\ &\quad \cdot \mathbf{S}_{CYL}^{--}(-\boldsymbol{\rho}_j, k, m_2, m') \cdot \mathbf{T}_{CS}^{--}(k, l' m'), \end{aligned}$$



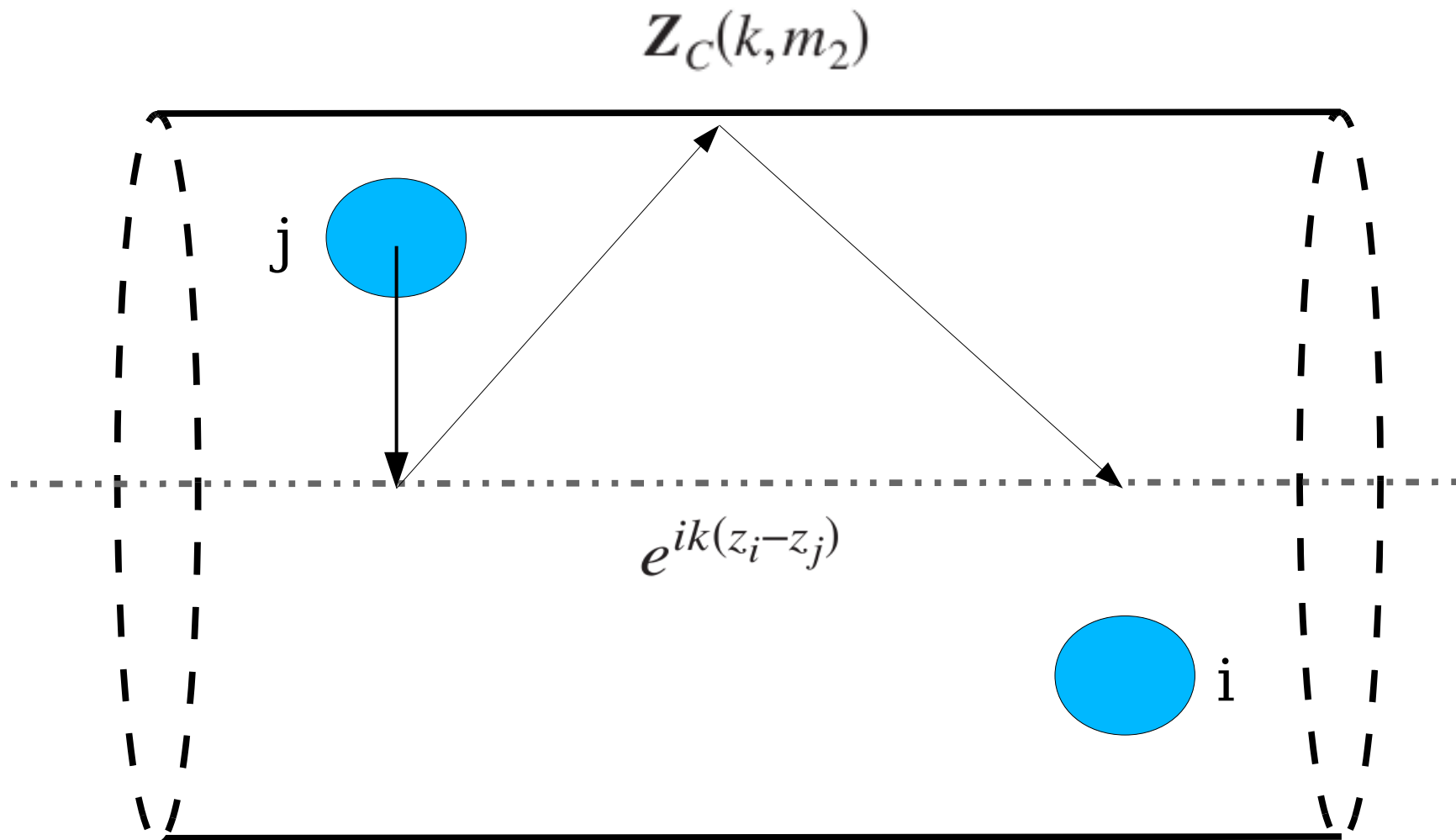
Metoda multipolowa



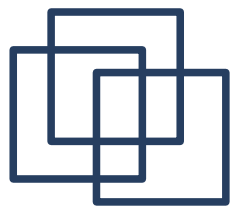
$$\mathbf{T}_{SC}^{++}(lm, k) \cdot \mathbf{S}_{CYL}^{++}(\rho_i, k, m, m_2) \cdot \mathbf{Z}_C(k, m_2) \cdot \mathbf{S}_{CYL}^{--}(-\rho_j, k, m_2, m') \cdot \mathbf{T}_{CS}^{--}(k, l' m')$$



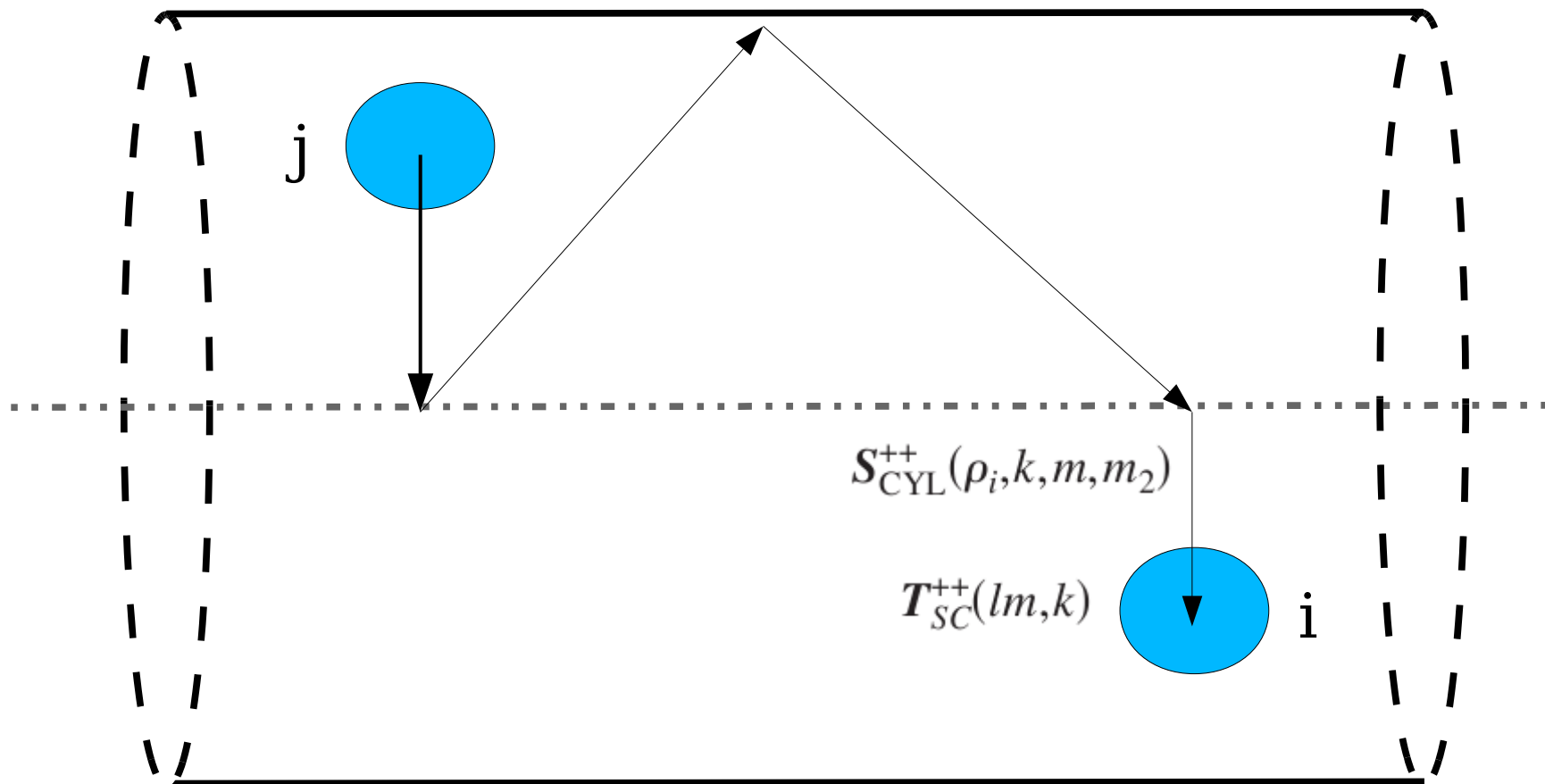
Metoda multipolowa



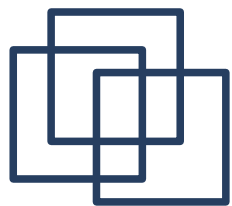
$$\mathbf{T}_{SC}^{++}(lm, k) \cdot \mathbf{S}_{CYL}^{++}(\rho_i, k, m, m_2) \cdot \mathbf{Z}_C(k, m_2) \cdot \mathbf{S}_{CYL}^{--}(-\rho_j, k, m_2, m') \cdot \mathbf{T}_{CS}^{--}(k, l' m')$$



Metoda multipolowa



$$T_{SC}^{++}(lm, k) \cdot S_{CYL}^{++}(\rho_i, k, m, m_2) \cdot Z_C(k, m_2) \cdot S_{CYL}^{--}(-\rho_j, k, m_2, m') \cdot T_{CS}^{--}(k, l' m')$$



Przykład - Macierz T^{++}

$$\begin{bmatrix} |v_{km0}^+\rangle \\ |v_{km1}^+\rangle \\ |v_{km2}^+\rangle \end{bmatrix}^T = \sum_l f(l,m|k) \begin{bmatrix} |v_{lm0}^+\rangle \\ |v_{lm1}^+\rangle \\ |v_{lm2}^+\rangle \end{bmatrix}^T \cdot \begin{bmatrix} k^{l-1} & 0 & 0 \\ 0 & k^l & 0 \\ 0 & 0 & k^{l+1} \end{bmatrix} \cdot \begin{bmatrix} 1 & s(l,m) & q(l,m) \\ 0 & 1 & s(l,m) \\ 0 & 0 & 1 \end{bmatrix}$$

$$\frac{1}{k} \left(-\frac{im}{\rho} I_m(|k|\rho) \mathbf{e}_\rho + \frac{dI_m(|k|\rho)}{d\rho} \mathbf{e}_\phi \right) e^{im\phi} e^{ikz} =$$

$$= \sum_l f(l,m) \left[(kr)^l \frac{1}{i(l+1)} \left(\frac{1}{\sin\theta} \partial_\phi Y_{lm} \mathbf{e}_\theta - \partial_\theta Y_{lm} \mathbf{e}_\phi \right) + s(l,m) (kr)^{l-1} \left(lY_{lm} \mathbf{e}_r + \partial_\theta Y_{lm} \mathbf{e}_\theta + \frac{1}{\sin\theta} \partial_\phi Y_{lm} \mathbf{e}_\phi \right) \right]$$

$$Y_l^m(\theta, \phi) = P_l^m(\cos\theta) e^{im\phi}$$

Funkcje specjalne:

$I_m(|k|\rho)$ - zmodyfikowane funkcje Bessela 1-ego rodzaju

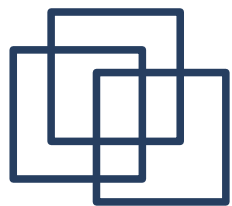
$K_m(|k|\rho)$ - zmodyfikowane funkcje Bessela 2-ego rodzaju

$P_l^m(\cos\theta)$ - stowarzyszone wielomiany Legendre'a

$$f(l,m|k) = \frac{(-1)^m i^{l-m} n_{lm}}{(l+m)!} [\text{sgn}(k)]^m$$

$$s(l,m) = -\frac{im}{l}$$

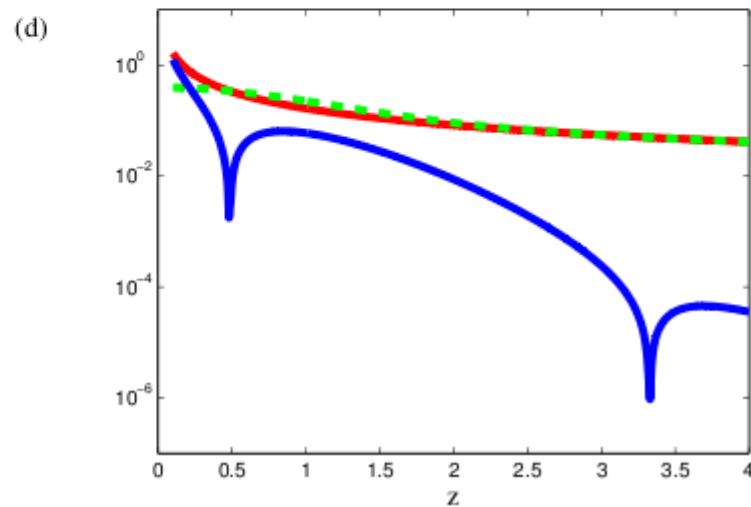
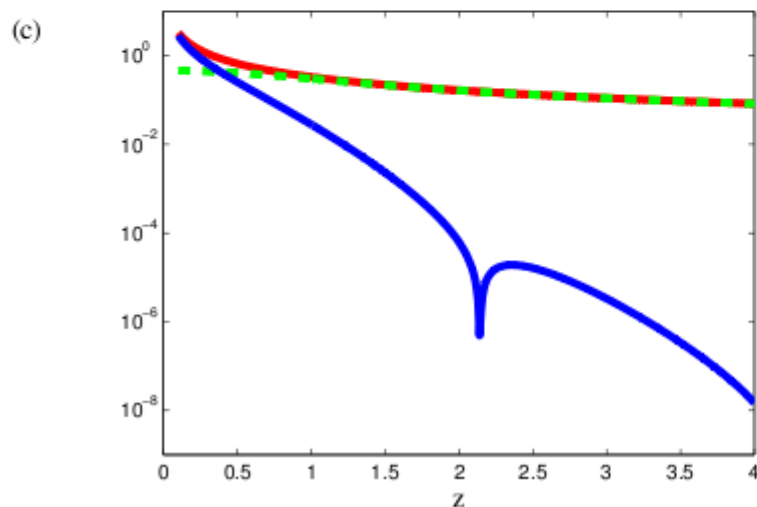
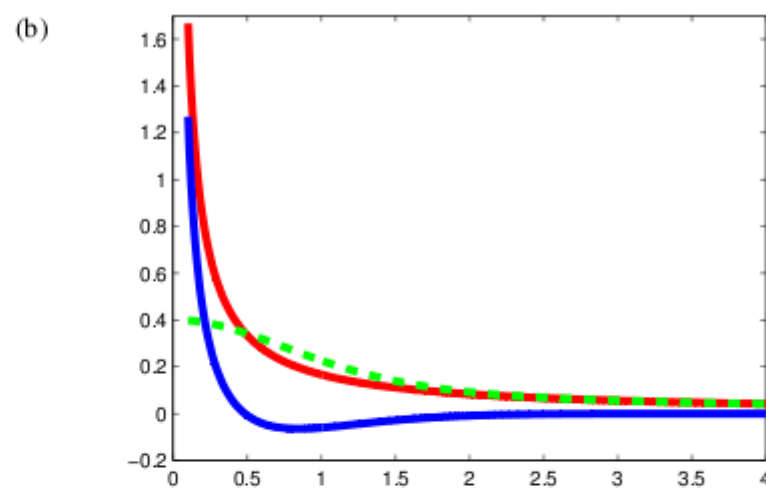
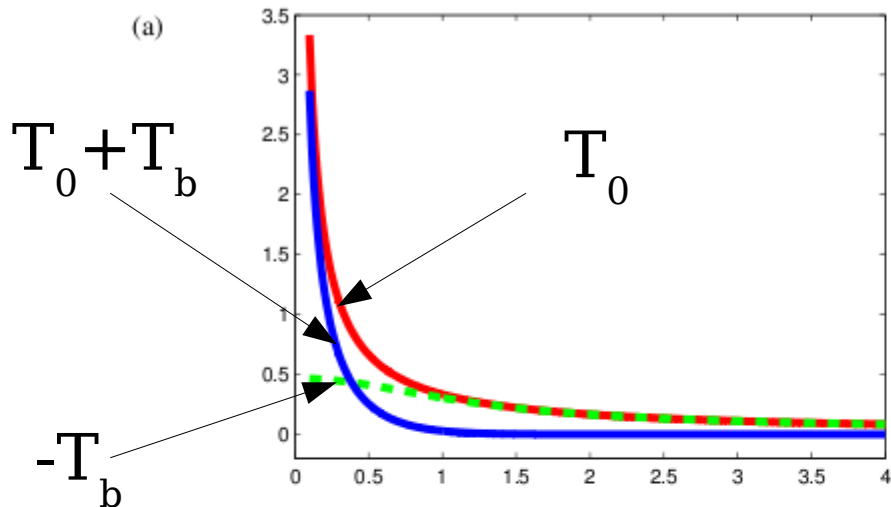
$$q(l,m) = \frac{l(l^2-l+1)+m^2(l-2)}{2l(2l-1)}$$



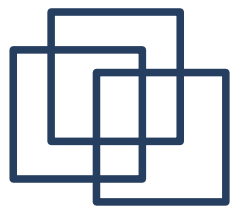
Wyniki obliczeń - elementy macierzowe w funkcji odległości

$$l = l' = 1, m = m' = 0, \sigma = \sigma' = 0$$

$$l = l' = 1, m = m' = 1, \sigma = \sigma' = 0$$

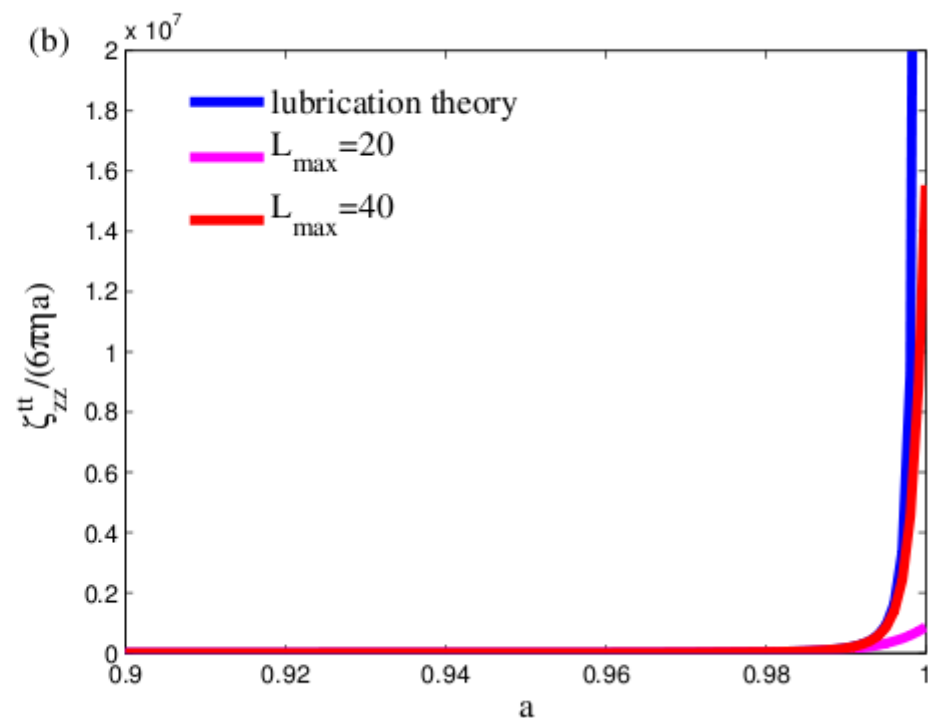
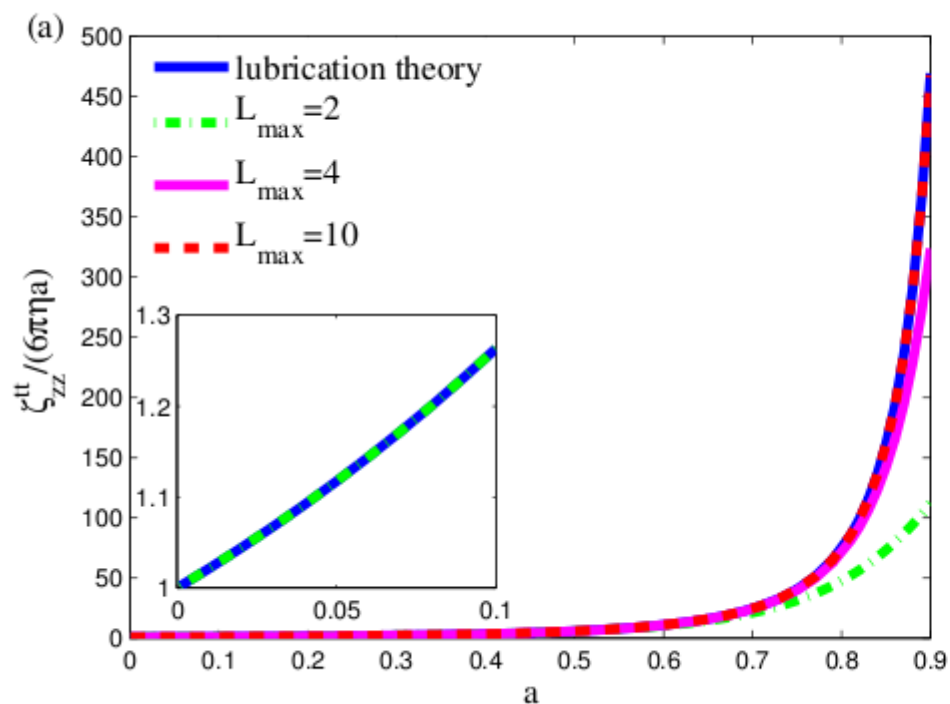


Kędzierski, Wajnryb, J. Chem. Phys 133, (2010)

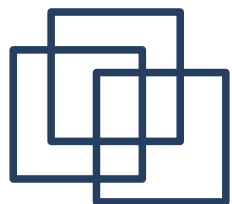


Wyniki obliczen

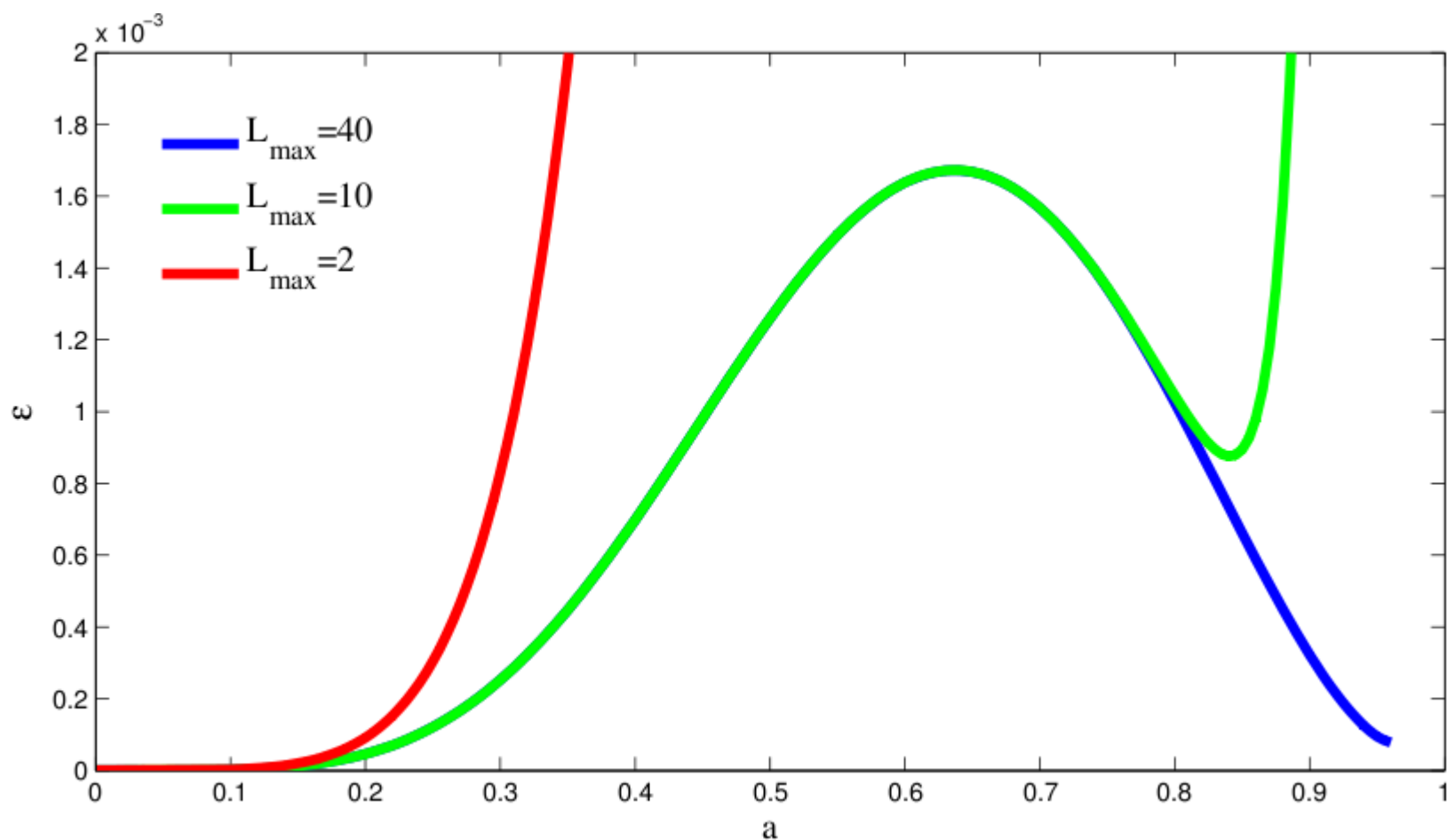
$$F_z = -\zeta_{zz}^{tt} U_z$$



Kędzierski, Wajnryb, J. Chem. Phys 133, (2010)



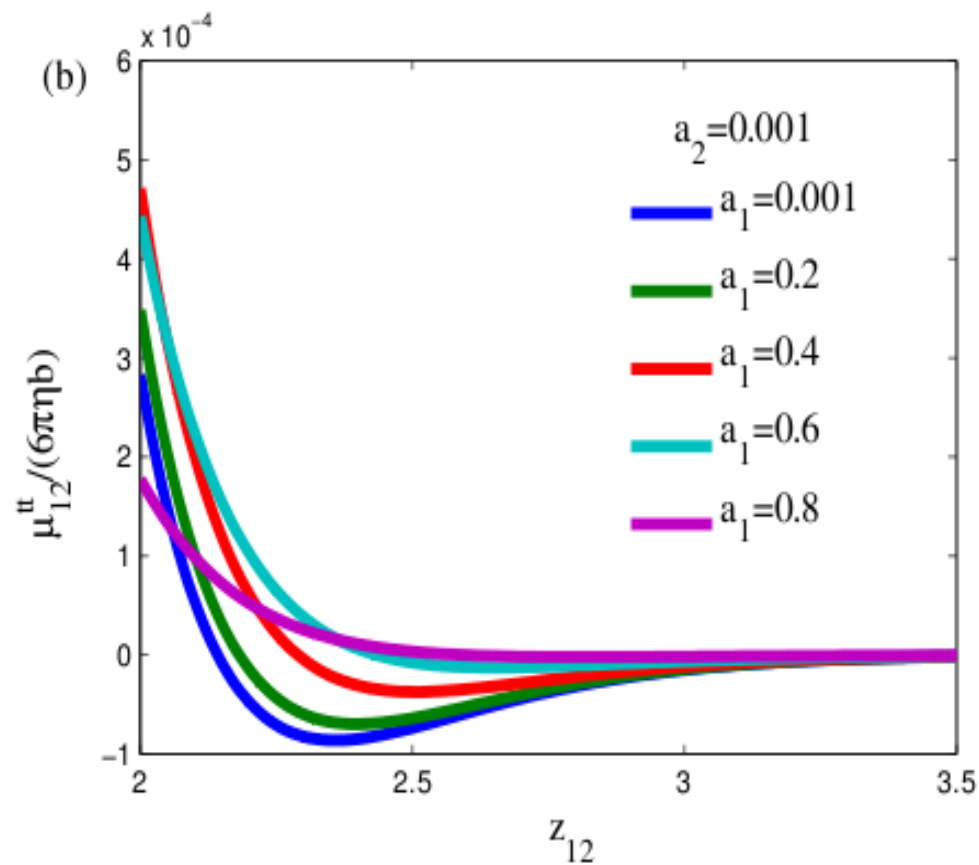
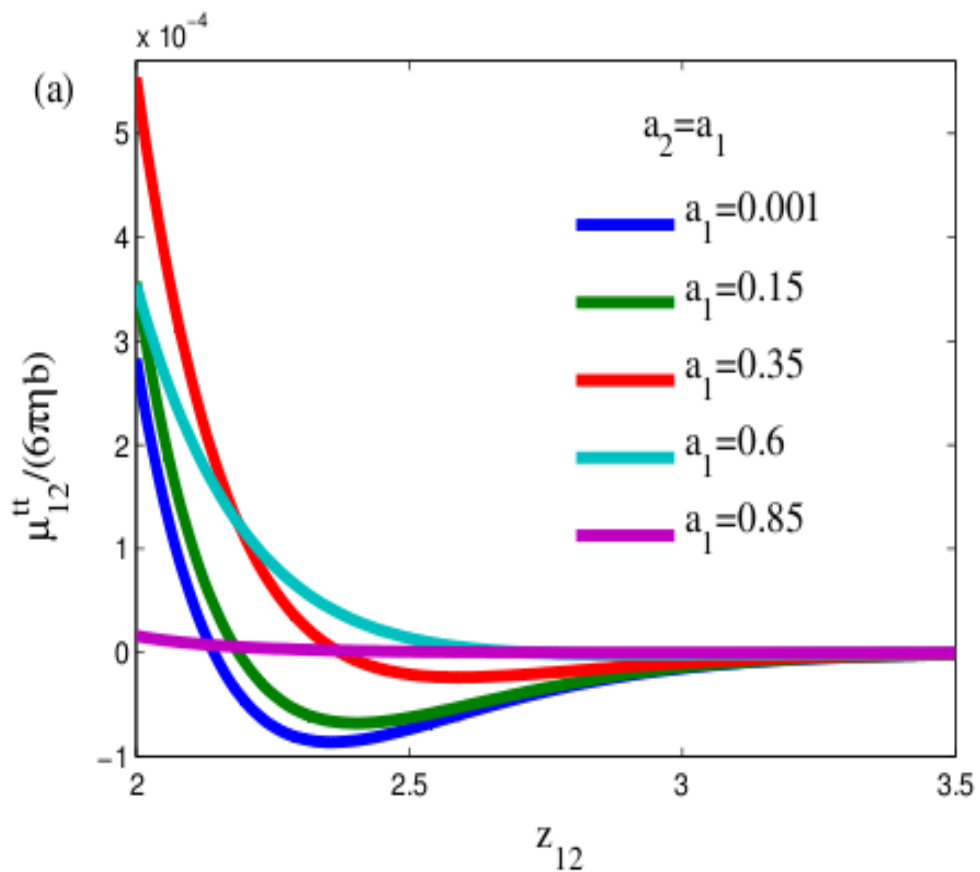
Wyniki obliczeń - błąd względny



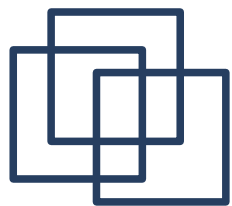
Kędzierski, Wajnryb, J. Chem. Phys 133, (2010)



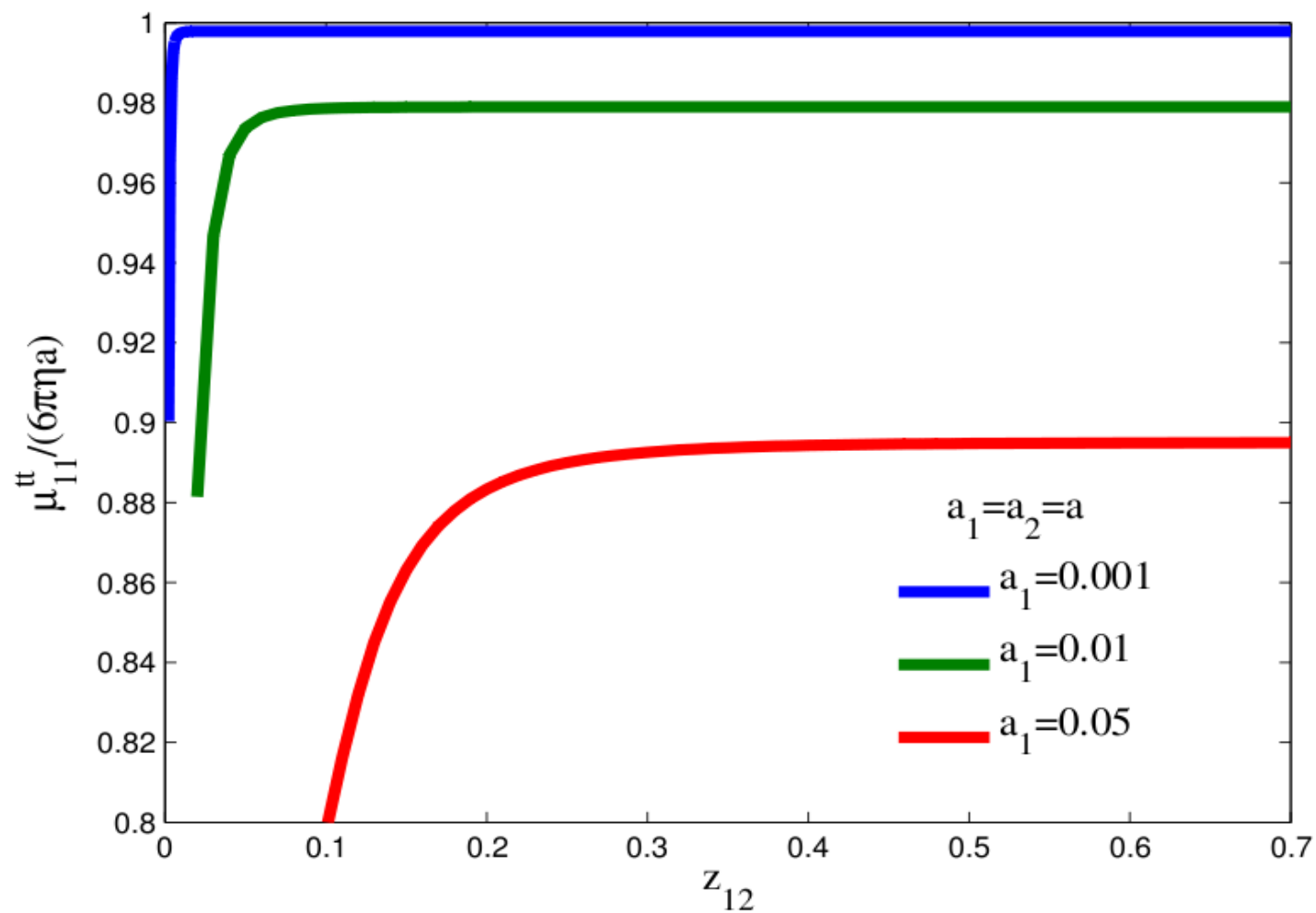
Wyniki obliczen - mobilność wzajemna



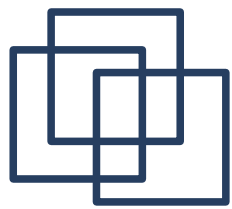
Kędzierski, Wajnryb, J. Chem. Phys 133, (2010)



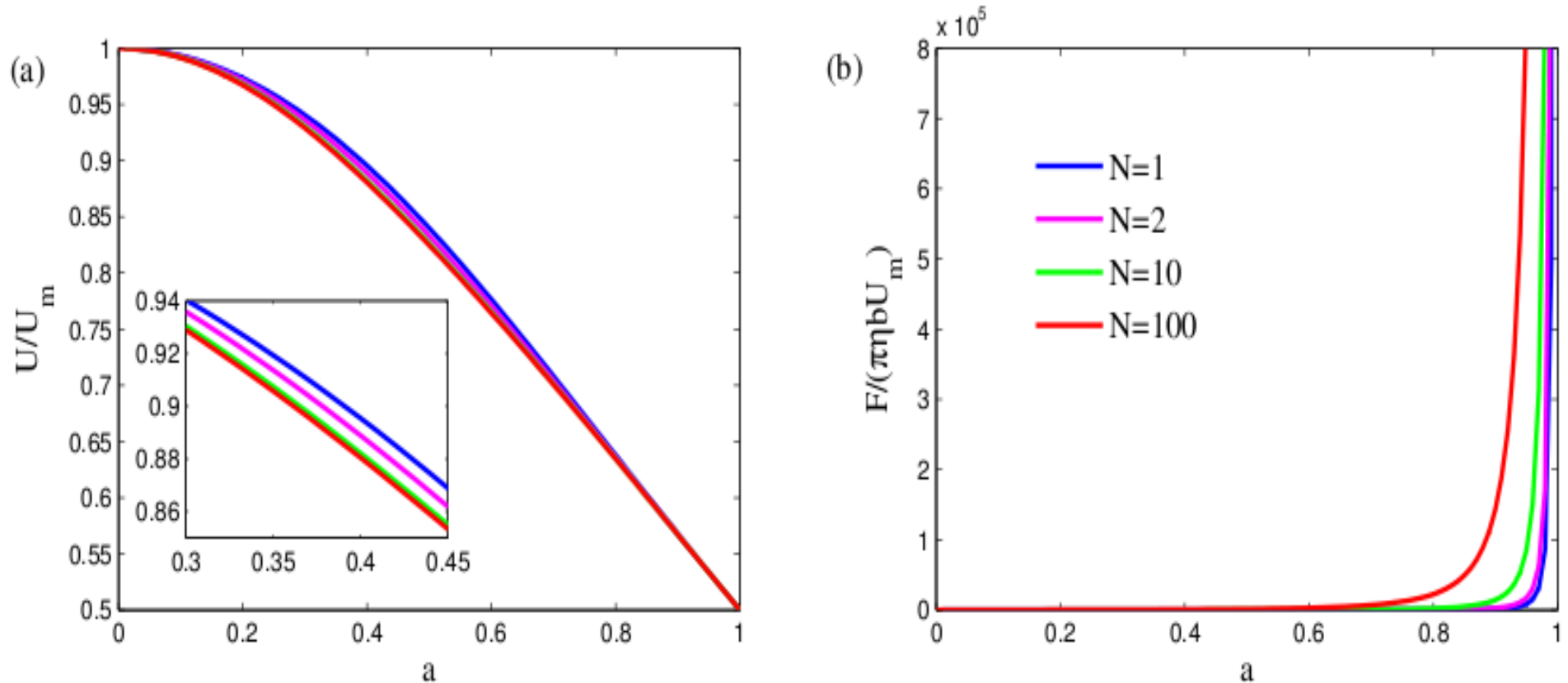
Wyniki obliczeń - mobilność własna



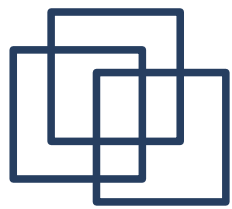
Kędzierski, Wajnryb, J. Chem. Phys 133, (2010)



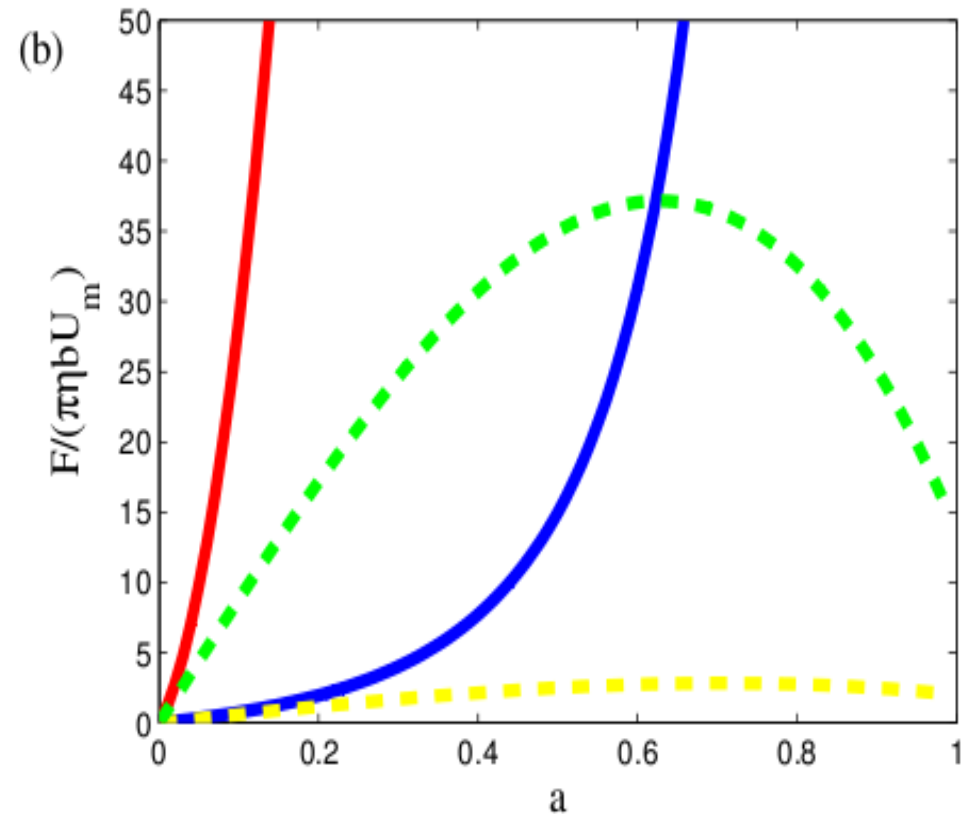
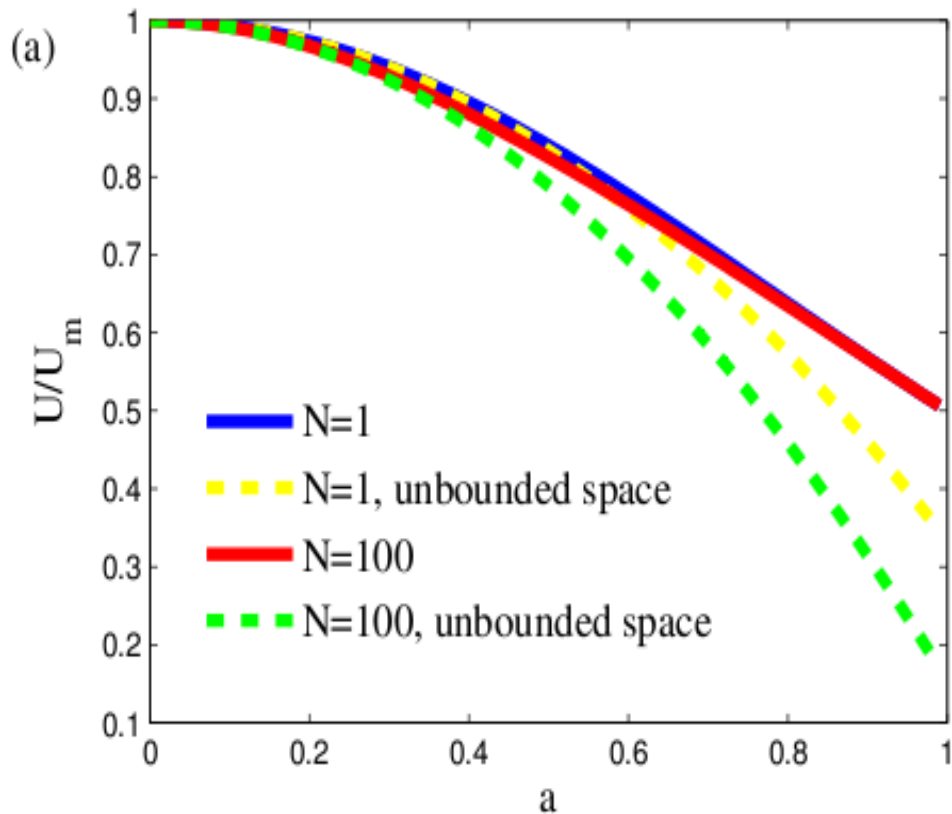
Wyniki obliczen - sztywny polimer w przeplywie parabolicznym



Kędzierski, Wajnryb, J. Chem. Phys 133, (2010)



Wyniki obliczen - sztywny polimer w przeplywie parabolicznym



Kędzierski, Wajnryb, J. Chem. Phys 133, (2010)