Geometry controlled dispersion in periodic corrugated channels

Matthieu Mangeat, Thomas Guérin and David S. Dean

Laboratoire Ondes et Matière d'Aquitaine, Université de Bordeaux, France

Introduction

- The dispersion in periodic channels was studied in two different regimes: for slowly varying channels where a dimensional reduction could be implemented and for highly corrugated channels where the first passage time between two narrow necks govern the dispersion.
- We use a general shape of symmetric channel, characterised by the radius as $R(z) = a + Hg(z/L)$, where $g(z/L) \in [0, 1]$.
- Two parameters appears: $\xi \equiv H/a$ and $\varepsilon \equiv a/L$.

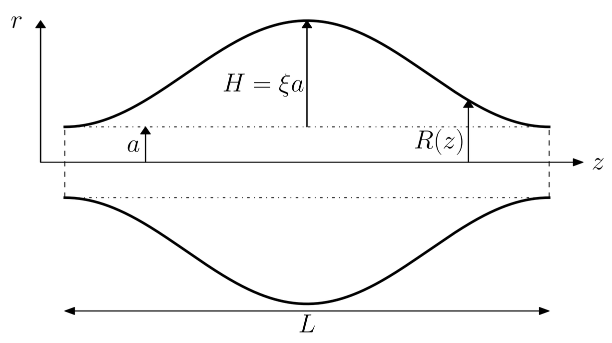

Figure 1 : Schematic of a channel.

- The long time effective diffusion coefficient $D_e \equiv \lim_{t\to\infty} \overline{[z(t)-z(0)]^2}/(2t)$ could be expressed as [1]

$$D_e = D_0 \left[1 + \frac{(d-1)\langle R' \, R^{d-2} \, f_S \rangle}{\langle R^{d-1} \rangle} \right]$$

where $\langle w \rangle = \int_0^L dz w(z)/L$ and $f_S(z) \equiv f(r = R(z), z)$. The function $f(r,z)$ satisfies the set of equations

$$\partial_z^2 f + r^{2-d} \partial_r [r^{d-2} \partial_r f] = 0$$

$$[R'(z)\partial_z f - \partial_r f]_{r=R(z)} = R'(z) \; ; \; f(r, z+L) = f(r,z) \; ; \; \partial_r f|_{r=0} = 0$$

Slowly varying channels ($\varepsilon \to 0$)

- Taking $R(z) = \varepsilon \tilde{R}(z)$, a standard perturbation in ε^2 brings the effective diffusivity. The existing developments was computed using a dimensional reduction carrying an effective one-dimensional diffusivity relied by the Lifson and Jackson formula [2] to the effective diffusivity D_e.

  - Fick-Jacobs [3]
  $$D_{\rm FJ} = \frac{D_0}{\langle \tilde{R}^{d-1} \rangle \langle \tilde{R}^{1-d} \rangle}$$
  - Reguera-Rubi [5]
  $$D_{\rm RR} = \frac{D_0}{\left\langle \tilde{R} \right\rangle \left\langle \tilde{R}^{-1} (1 + \varepsilon^2 \tilde{R}'^2)^{\gamma} \right\rangle}$$
  - Zwanzig [4]
  $$D_{\rm Zw} = \frac{D_0}{\langle \tilde{R} \rangle \left[\langle \tilde{R}^{-1} \rangle + \gamma \varepsilon^2 \langle \tilde{R}'^2 / \tilde{R} \rangle \right]}$$
  - Kalinay-Percus [6]
  $$D_{\rm KP} = \frac{D_0}{\left\langle \tilde{R} \right\rangle \left\langle \frac{\varepsilon \tilde{R}'}{\tilde{R} \arctan(\varepsilon \tilde{R}')} \right\rangle}$$

- These results are only correct at the order ε^2. A more general expansion was given by [6, 7] as

$$D_e = D_{\rm FJ} \left[1 + C_2 \varepsilon^2 + C_4 \varepsilon^4 + C_6 \varepsilon^6 + \mathcal{O}(\varepsilon^8) \right],$$

where C_2, C_4 and C_6 are functions of $\tilde{R}$ and its derivatives depending on the dimension. The function $f(r,z)$ behaves as

$$f(r,z) \underset{\varepsilon \to 0}{=} f(z).$$

Wide channels ($\varepsilon \to \infty$)

- In the limit of large ε, the previous results are not correct and a one-dimensional reduction is not possible. Here, the effective diffusivity can be seen as the rate of time spent in the region $r < a$, which yields with ergodicity to

$$\frac{D_e}{D_0} \underset{\varepsilon \to \infty}{=} \frac{V(r<a)}{V} = \frac{a^{d-1}}{\langle R^{d-1} \rangle}.$$

- Solving the equations at the leading order of the ε^{-1} expansion gives

$$f(r,z) \underset{\varepsilon \to \infty}{=} z \, \theta(r-a) L + b(r),$$

which implies the presence of a boundary layer at $r = a$. We define the boundary layer coordinate η as $r = a + \eta L$ and the function $f(\eta, z)$ satisfies the Laplace equation and after some conformal transformations we get

$$f(\eta, z) = \mathrm{Re} \left[\frac{iL}{\pi} \ln \left(1 + \sqrt{1 + e^{-2\pi i z/L + 2\pi\eta}} \right) \right] + b(a).$$

- The ε^{-1} contribution of the effective diffusivity given by the boundary layer term do not depend on the channel geometry,

$$D_e = D_0 \frac{a^{d-1}}{\langle R^{d-1} \rangle} \left[1 + \frac{(d-1)\ln 2}{\pi \varepsilon} + \mathcal{O}(\varepsilon^{-2}) \right].$$

Padé type approximant and numerical results

- We develop a Padé type approximant statisfying both limits $\varepsilon \to 0$ and $\varepsilon \to \infty$ such that

$$D_e = D_{\rm FJ} \frac{1 + a_1 \varepsilon + a_2 \varepsilon^2 + a_3 \varepsilon^3}{1 + b_1 \varepsilon + b_2 \varepsilon^2 + b_3 \varepsilon^3}.$$

- The numerical results for the bidimensional channel of radius $R(z) = \varepsilon\{0.5 + 0.266[\cos(2\pi z) + \sin(6\pi z)]\}$ shows a good approximation of the effective diffusivity by the Padé development.

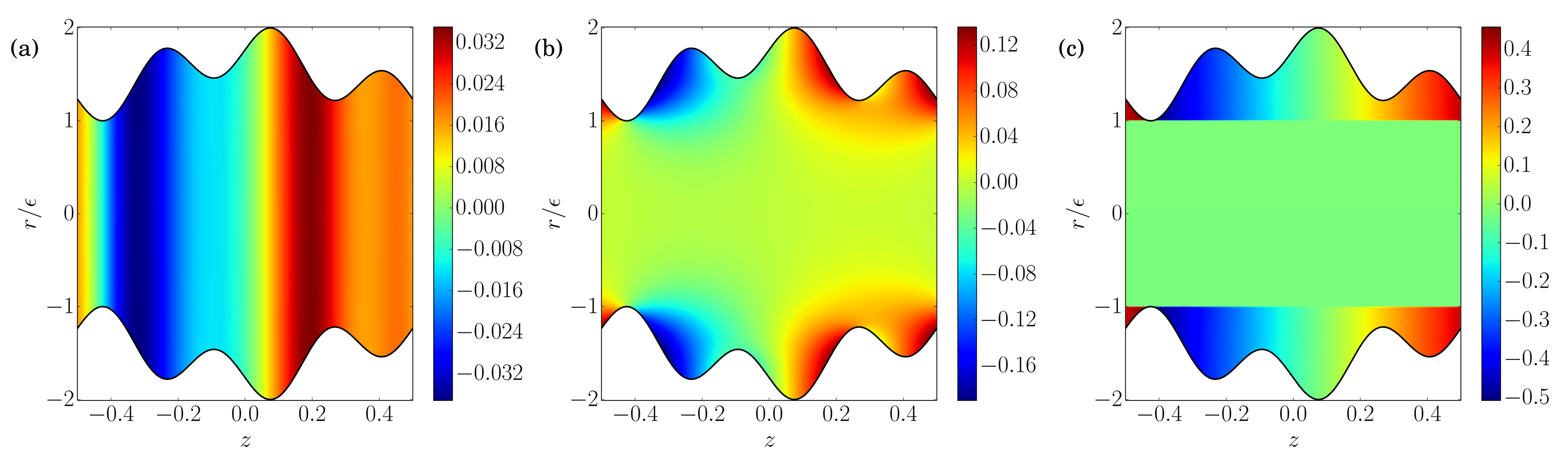

Figure 2 : The exact solution $f(r,z)$ for (a) $\varepsilon = 0.01$ (FJ) , (b) $\varepsilon = 0.5$ et (c) $\varepsilon = 100$ (WC).

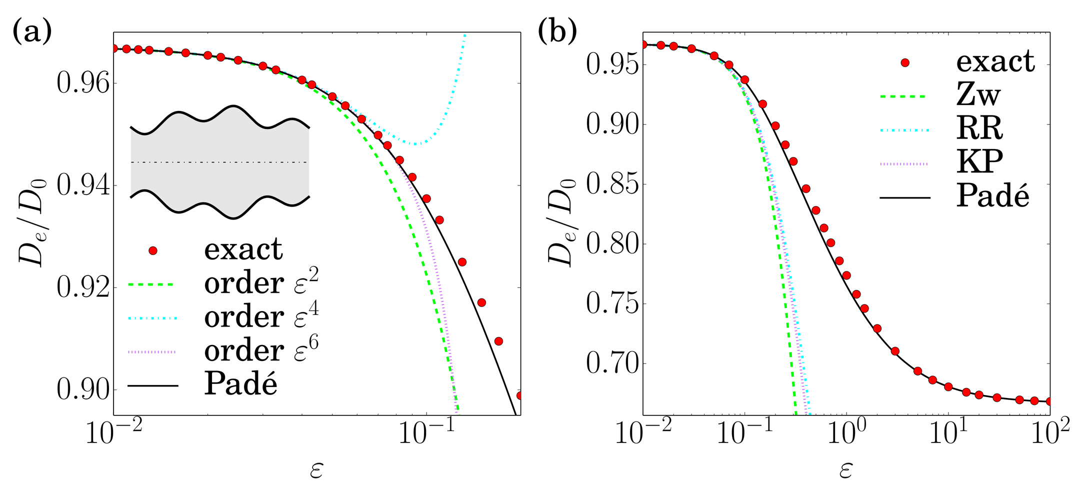

Figure 3 : Padé development versus exact solution given by a PDE solver. (a) The domain of slowly varying channels with the successive terms of the perturbative expansion in ε^2. (b) Comparison with the existing developments [4, 5, 6] with finite values of ε.

Intermediate regime of dispersion

- The Padé development is not correct in an intermediate range of ε, which grows in the large ξ limit. A small pore openings perturbation [8, 9] can solve this case. The effective diffusivity reads as

$$D_e \simeq \frac{L^2 D_0}{V} \times \begin{cases} \frac{\pi}{2\ln(2\kappa/\varepsilon)} & (d=2) \\ 2a & (d=3) \end{cases}$$

where κ is a constant depending on the ratio H/L and the shape of the channel as

$$\ln \kappa = \frac{\pi}{2} [R(\mathbf{r}_0, \mathbf{r}_0) + R(\mathbf{r}_1, \mathbf{r}_1) - 2G(\mathbf{r}_0, \mathbf{r}_1)],$$

where G is the pseudo-Green's function of the domain without opening, R is the non-diverging part of this Green's function and $\mathbf{r}_0, \mathbf{r}_1$ are the positions of the openings. In the limit $H \gg L$, $\kappa = 2/\pi$.

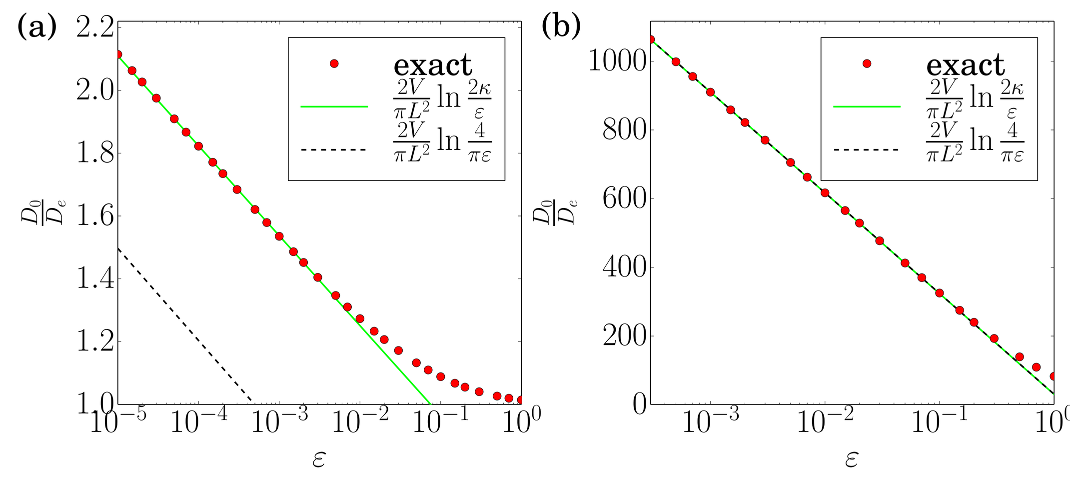

Figure 4 : Effective diffusivity D_e for channel of ellipsoidal shape $g(u) = \sqrt{1 - 4u^2}$ with (a) $H = 0.1L$ and (b) $H = 100L$ in presence of small openings.

- Comparing with [9] : $D_e = L^2/(2T)$ where T is the time to reach a pore, starting from the opposite opening considered as reflecting.

Highly corrugated channels and validity diagrams

- The range of the intermediate regime depends on the geometry close to the minimum radius of the channel, chosen to be at $z = 0$, such that

$$R(z \to 0) \simeq a(1 + A\xi|z|^{\nu}).$$

- For $\nu < \nu_c \equiv \frac{1}{d-1}$, $D_{\rm FJ}$ is finite and independant of ε and ξ,

$$D_{\rm FJ} = \frac{D_0}{\langle g^{d-1} \rangle \langle g^{1-d} \rangle}.$$

The dispersion through small openings is controlled by the narrow escape time (NET).

- For $\nu > \nu_c$, $\langle g^{1-d} \rangle$ diverges and $D_{\rm FJ}$ vanishes with increasing ξ as

$$D_{\rm FJ} = \frac{L^2}{2T} \sim D_0 \xi^{1/\nu - d + 1}.$$

The dispersion through small openings is controlled by events of narrow escape through a funnel (NEF).

- A diagram (ε, ξ) summarizing the asymptotic estimates of D_e is given for both smooth ($\nu > \nu_c$) and highly corrugated ($\nu < \nu_c$) channels.

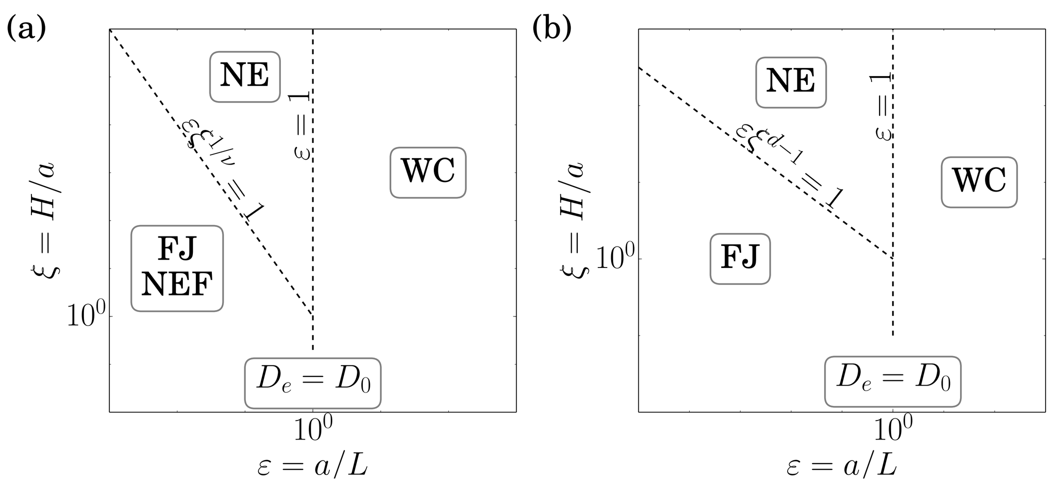

Figure 5 : The validity diagrams of D_e expressions for (a) $\nu > \nu_c$ and (b) $\nu \leq \nu_c$.

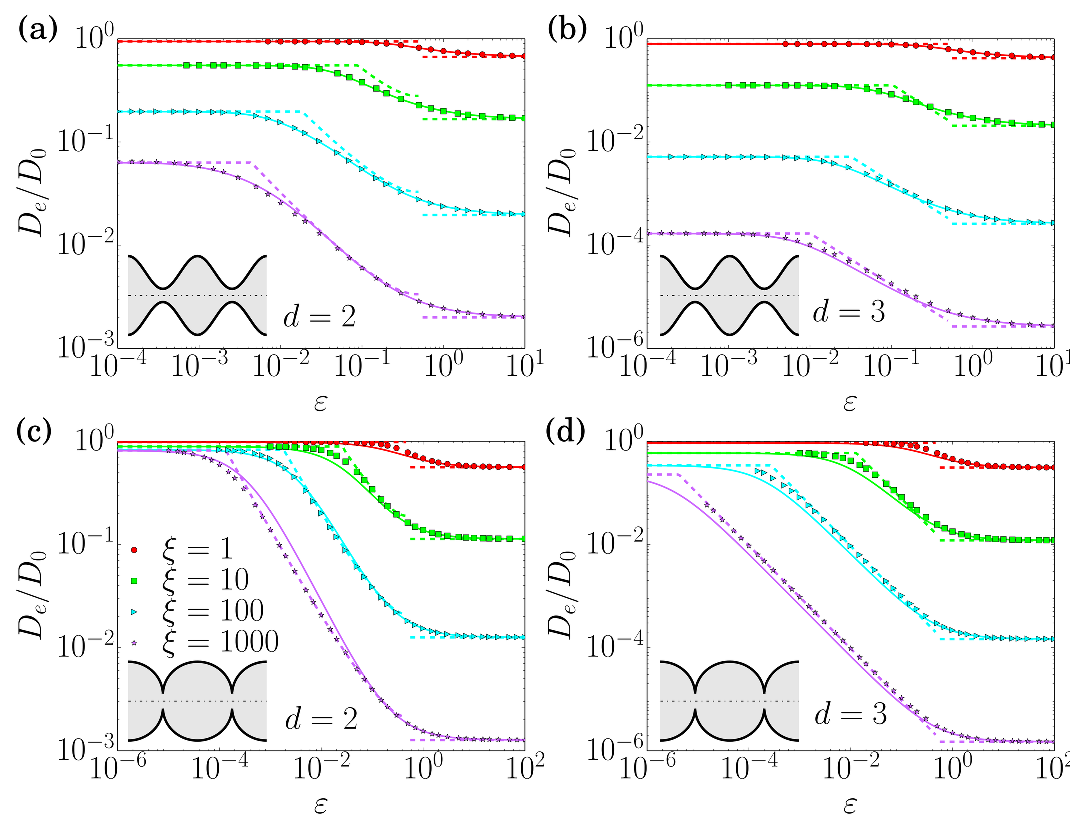

Figure 6 : Effective diffusivity D_e for channels of sinusoidal shape $g(u) = [1 + \cos(2\pi u)]/2$ ($\nu = 2$) in 2D (a) and 3D (b), and ellipsoidal shape $g(u) = \sqrt{1 - 4u^2}$ ($\nu = 0.5$) in 2D (c) and 3D (d). Disks represent the numerical solution, continuous lines correspond to the Padé approximant and dashed lines represent the various asymptotic regimes: FJ, NET and WC with increasing ε.

- We identify all mechanisms which control the dispersion in a symmetric channel and the domain of validity of the asymptotic expressions of the long time effective diffusivity in terms of (ε, ξ) parameters.

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