Mapping of diffusion in quasi-1D systems onto the longitudinal coordinate

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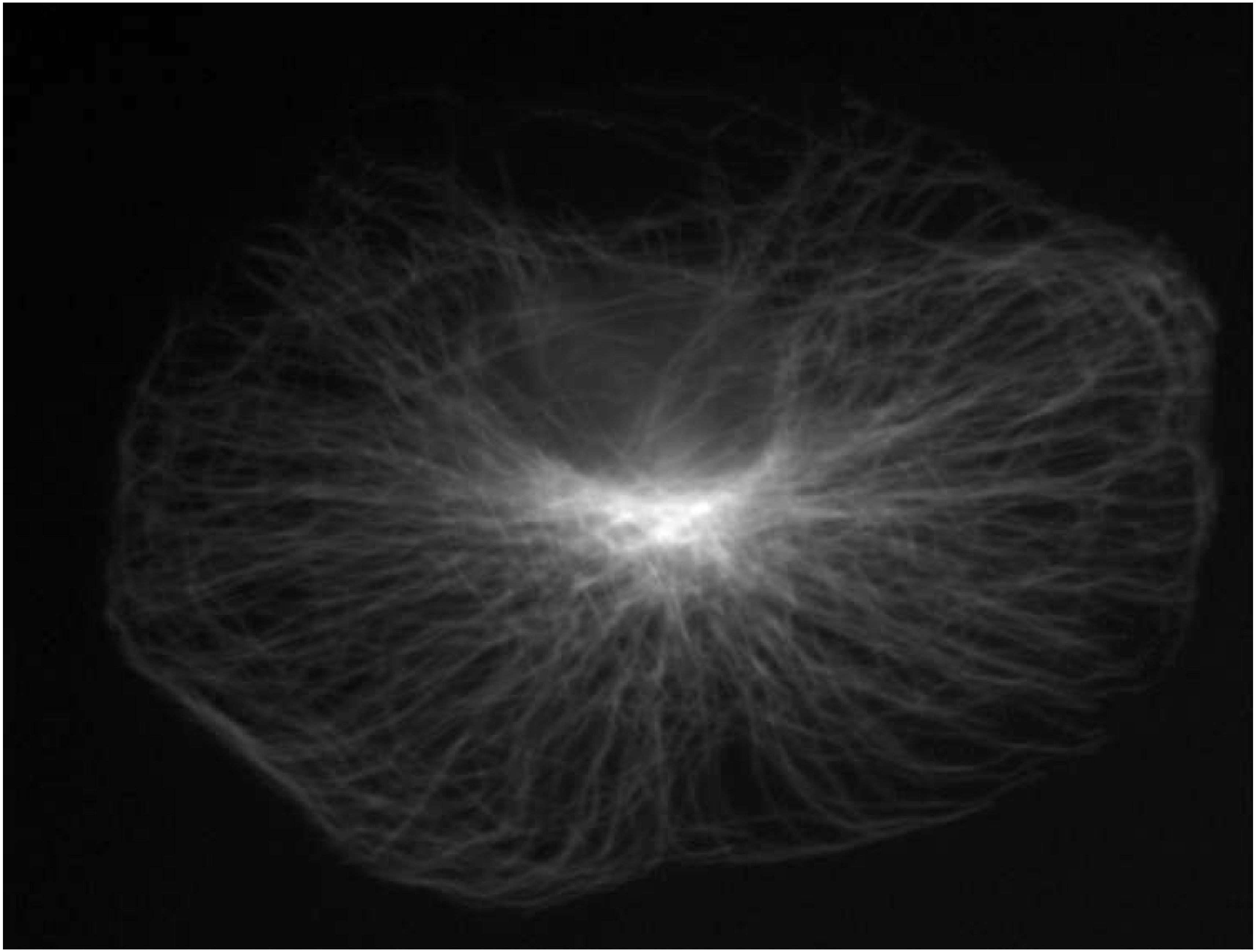
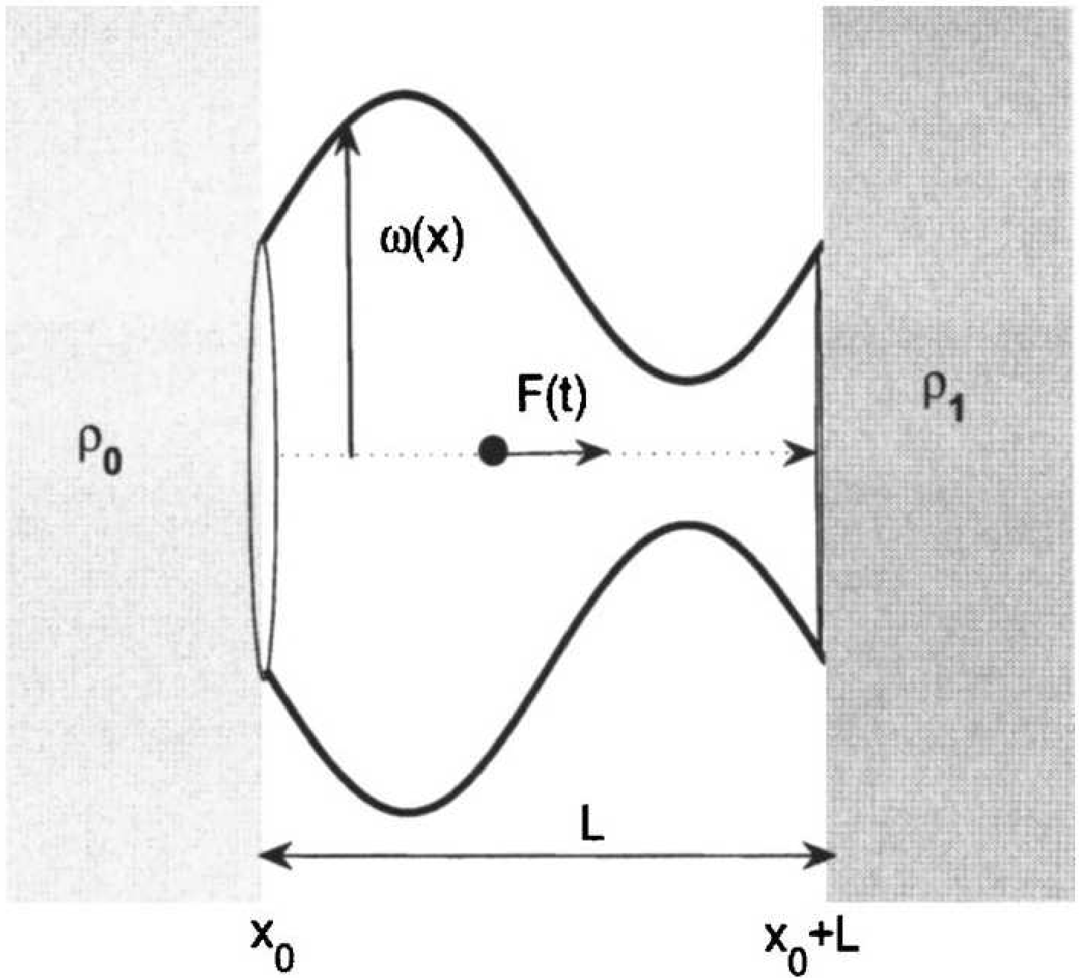
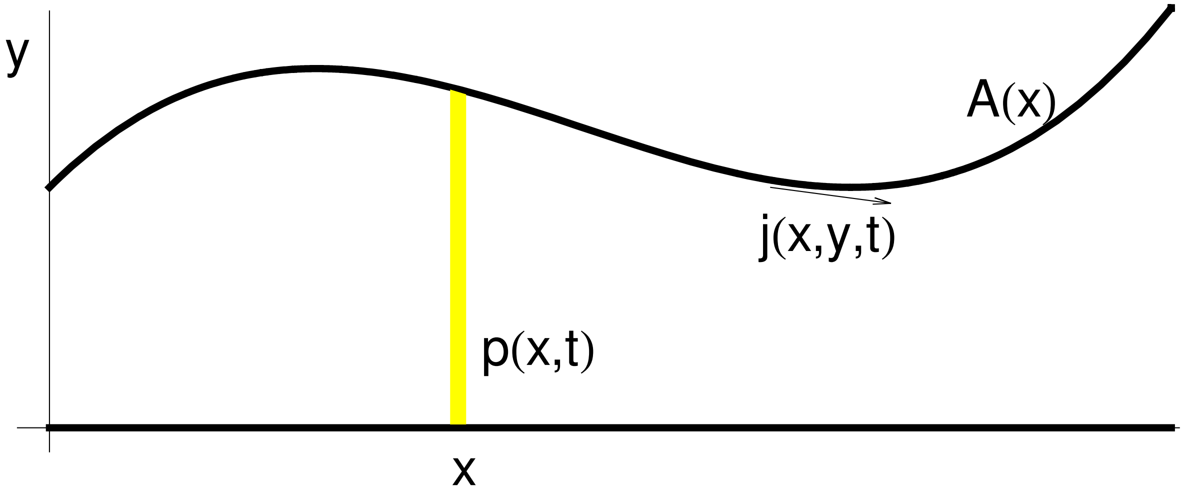


Brownian pumps



Diffusion in a 2D channel



$$\big(\partial_t - D\Delta\big)\rho(x,y,t) = 0$$

$+$ Neumann BCs:

$$\partial_y \rho = 0\Big|_{y=0} \quad \text{and}$$
$$\partial_y \rho = A' \partial_x \rho\Big|_{y=A(x)}$$

as the current density $\mathbf{j}(x,y,t) = -D\nabla\rho(x,y,t)$ at the hard walls is parallel to them.

Is there any corresponding equation for $\quad p(x,t) = \displaystyle\int_0^{A(x)} \rho(x,y,t)dy$?

Exact formulation: the 1D density $p(x,t)$ is determined by

the diffusion equation + BCs + an initial condition $\rho(x,y,0) = \rho_0(x,y)$.
We can:

↙ ↘

- either to solve the 2D problem
- and to map the solution $\rho(x,y,t)$

$$p(x,t) = \int_0^{A(x)} \rho(x,y,t)dy$$

- or to map the initial condition
- and to solve some equation

$$\frac{\partial p(x,t)}{\partial t} = \hat{Q}(x,\partial_x)p(x,t)$$

Our goal:

to find the operator $\hat{Q}(x,\partial_x)$ to make both treatments equivalent.

The simplest approximations:

$$\text{Fick} - \text{Jacobs equation}: \qquad \frac{\partial p(x,t)}{\partial t} = D\frac{\partial}{\partial x}A(x)\frac{\partial}{\partial x}\,\frac{p(x,t)}{A(x)} \quad ,$$

$$\text{Zwanzig's correction (1992)}: \qquad \frac{\partial p(x,t)}{\partial t} = D\frac{\partial}{\partial x}A(x)\left(1-\frac{1}{3}A'^2(x)\right)\frac{\partial}{\partial x}\frac{p(x,t)}{A(x)}$$

Reguera and Rubí (2001) concluded from the non-equilibrium TD

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}A(x)D(x)\frac{\partial}{\partial x}\,\frac{p(x,t)}{A(x)}$$

$$\text{with } D(x) \text{ estimated as} \qquad D(x) \simeq \Big(1 + A'^2(x)\Big)^{-1/3} \quad .$$

Trick $\#1$: suppose anisotropy of the diffusion constant D

$$\frac{\partial\rho(x,y,t)}{\partial t} = \Big(D_x\frac{\partial^2}{\partial x^2} + D_y\frac{\partial^2}{\partial y^2}\Big)\rho(x,y,t)\ ; \qquad D_y \gg D_x$$

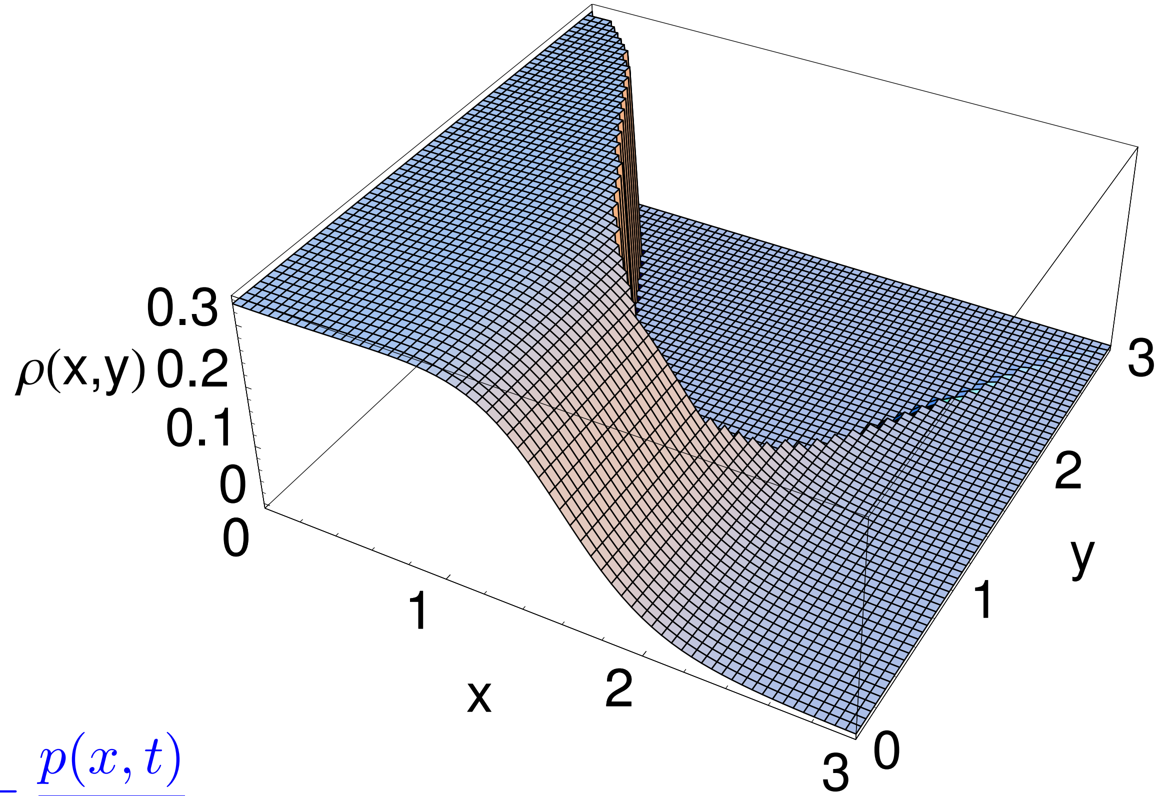
Rescaling time $D_x t \to t \ \Rightarrow$ we introduce a small parameter $\epsilon = D_x/D_y$;

$$\Big(\frac{\partial}{\partial t}-\frac{\partial^2}{\partial x^2}-\frac{1}{\epsilon}\frac{\partial^2}{\partial y^2}\Big)\rho(x,y,t) = 0\,; \quad \Big(\frac{\partial}{\partial y}-\epsilon A'(x)\frac{\partial}{\partial x}\Big)\rho(x,y,t)\Big|_{y=A(x)} = 0\,.$$

After integration of the diffusion equation over y and using BC:

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial^2 p(x,t)}{\partial x^2} - \frac{\partial}{\partial x}\Big(A'(x)\ \rho(x,A(x),t)\Big)$$

Zero-th order, $\epsilon \to 0$:



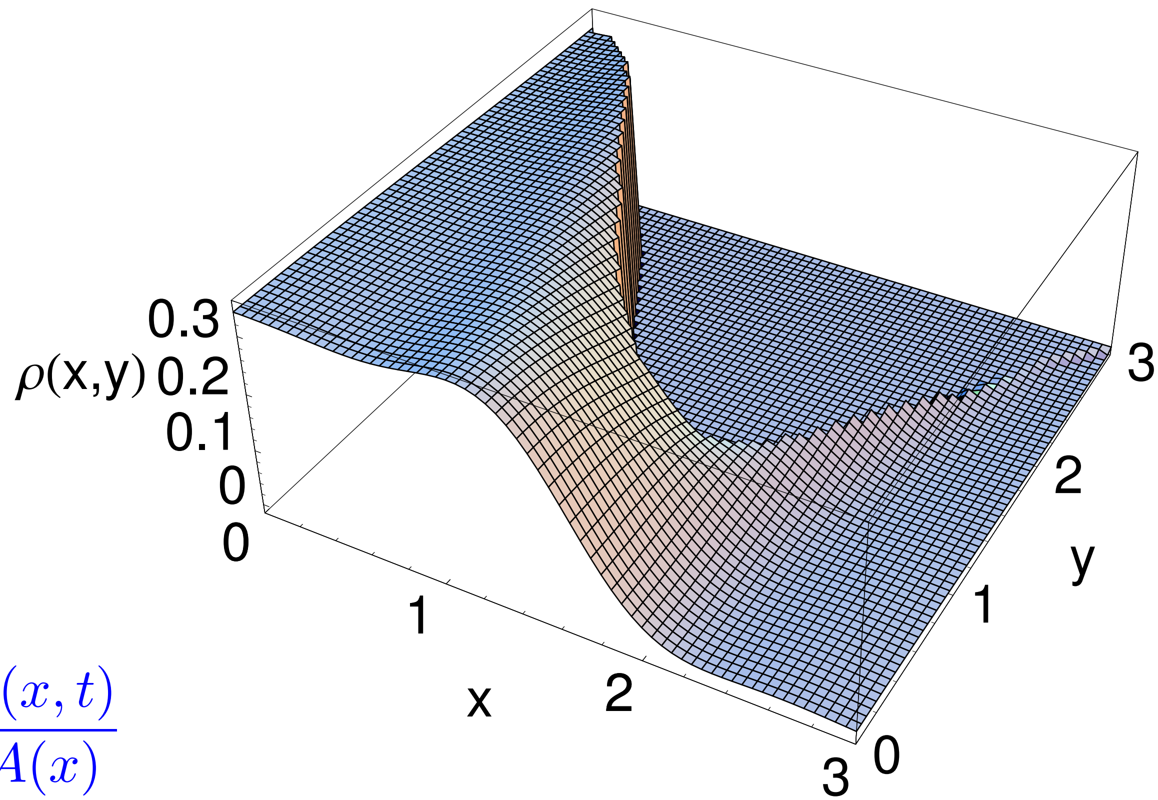
- transverse relaxation is so fast that $\rho(x, y, t)$ is flat in the transverse direction;

$$\rho(x, y, t) = \rho(x, A(x), t) = \frac{p(x, t)}{A(x)} \,.$$

Then

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial^2 p(x,t)}{\partial x^2} - \frac{\partial}{\partial x}\left(A'(x)\frac{p(x,t)}{A(x)}\right) = \frac{\partial}{\partial x}A(x)\frac{\partial}{\partial x}\frac{p(x,t)}{A(x)} \quad = \mathrm{FJ\ eq.}$$

For $\epsilon > 0$:



- transverse relaxation is slower;

ρ becomes curved in the transverse direction;

$$\rho(x,y,t) = \hat{\omega}(x,y,\partial_x)\frac{p(x,t)}{A(x)}$$

- this is substituted for $\rho(x, A(x), t)$ in the mapped equation:

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial^2 p(x,t)}{\partial x^2} - \frac{\partial}{\partial x}\Big(A'(x)\ \hat{\omega}(x, A(x), \partial_x)\frac{p(x,t)}{A(x)}\Big)$$

Trick $\#2$: search for the operator of backward mapping $\hat{\omega}$

a) $\hat{\omega}$ does not depend on time, hence $\frac{\partial}{\partial t}\,\hat{\omega}(x,y,\partial_x) = \hat{\omega}(x,y,\partial_x)\,\frac{\partial}{\partial t}$

b) $\hat{\omega}$ satisfies the inverse (unity) relation

$$\frac{1}{A(x)}\int_0^{A(x)} dy\,\hat{\omega}(x,y,\partial_x)\frac{p(x,t)}{A(x)} = \frac{p(x,t)}{A(x)} \qquad \text{for any solution } p(x,t),$$

c) $\hat{\omega}$ can be expanded in ϵ : $\qquad \hat{\omega}(x,y,\partial_x) = 1+\sum_{j=1}^{\infty}\epsilon^j\hat{\omega}_j(x,y,\partial_x)$

d) the backward mapped $\rho(x,y,t) = \hat{\omega}(x,y,\partial_x)\big[p(x,t)/A(x)\big]$ solves the diffusion equation

$$\sum_{j=0}^{\infty} \epsilon^{j+1}\Big(\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2} - \frac{1}{\epsilon}\frac{\partial^2}{\partial y^2}\Big)\hat{\omega}_j(x,y,\partial_x)\frac{p(x,t)}{A(x)} = 0$$

with Neumann BC at $y = 0$ and $A(x)$.

$$\frac{\partial p(x,t)}{\partial t} = \hat{Q}(x,\partial_x)p(x,t) = \frac{\partial}{\partial x}\Big[\frac{\partial}{\partial x}A(x) - A'(x)\hat{\omega}(x,A(x),\partial_x)\Big]\frac{p(x,t)}{A(x)}$$

$$= \frac{\partial}{\partial x}A(x)\Big(1 - \epsilon\hat{Z}(x,\partial_x)\Big)\frac{\partial}{\partial x}\,\frac{p(x,t)}{A(x)}\ ,$$

where also $\hat{Z}$ can be expanded in ϵ : $\qquad \epsilon\hat{Z}(x,\partial_x) = \sum_{j=1}^{\infty}\epsilon^j\hat{Z}_j(x,\partial_x)\ .$

Recurrence relations:

$$\frac{\partial^2}{\partial y^2}\,\hat{\omega}_{j+1}(x,y,\partial_x) = -\frac{\partial^2}{\partial x^2}\,\hat{\omega}_j(x,y,\partial_x) - \sum_{k=0}^{j}\hat{\omega}_{j-k}(x,y,\partial_x)\frac{1}{A(x)}\,\frac{\partial}{\partial x}A(x)\hat{Z}_k(x,\partial_x)\frac{\partial}{\partial x}$$

and $$\hat{Z}_j(x,\partial_x)\frac{\partial}{\partial x} = \frac{A'(x)}{A(x)}\,\hat{\omega}_j(x,A(x),\partial_x) \qquad \text{for } j>0.$$

- we start from $\hat{\omega}_0(x,y,\partial_x) = 1$ and $\hat{Z}_0(x,\partial_x) = -1$ (valid for FJ)

- use BC and the inverse relation for fixing the integration constants at double integration of $\partial_y^2\hat{\omega}_{j+1}(x,y,\partial_x)$

Resultant expansions of $\hat{\omega}(x, y, \partial_x)$ and $\hat{Z}(x, \partial_x)$:

$$\hat{\omega}(x, y, \partial_x) = 1 + \epsilon \left(3y^2 - A'^2(x)\right) \frac{A'(x)}{6A(x)} \frac{\partial}{\partial x} + \ldots$$

and

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x} A \Big[1 - \frac{\epsilon}{3} A'^2 - \frac{\epsilon^2}{45} A' \Big(2A\big(AA'\big)' \frac{\partial}{\partial x} + + AA'A'' + A^2 A^{(3)} - 7A'^3 \Big) + \ldots \Big] \frac{\partial}{\partial x} \frac{p(x,t)}{A(x)}$$

Instead of the **function** $D(x)$, we get an **operator** containing $\partial / \partial x$.

Stationary flow: $D(x)$ can be expressed using $\hat{Z}$.

Any form of the equation for $\partial_t p(x,t)$ represents 1D mass conservation law.

$$J(x,t) = -A(x)D(x)\frac{\partial}{\partial x}\frac{p(x,t)}{A(x)}\,; \quad J(x,t) = A(x)\Big(1 - \epsilon\hat{Z}(x,\partial_x)\Big)\frac{\partial}{\partial x}\frac{p(x,t)}{A(x)}$$

In the stationary state: J(x,t)=J constant;

– any stationary solution $p(x)$ has to keep $\quad \dfrac{\partial}{\partial x}\dfrac{p(x)}{A(x)} = \dfrac{-J}{A(x)D(x)}\,.$

Final relation:

$$\frac{1}{D(x)} = A(x)\Big[1 - \epsilon\hat{Z}(x,\partial_x)\Big]^{-1}\frac{1}{A(x)}$$

enables us to generate $D(x)$ as an expansion in ϵ.

$$D(x) = 1 - \frac{\epsilon}{3} A'^2 + \frac{\epsilon^2}{45}\Big(9A'^4 + AA'^2A'' - A^2A'A^{(3)}\Big) - \frac{\epsilon^3}{945}\Big(135A'^6 + 45AA'^4A''$$

$$-58A^2A'^2A''^2 - 41A^2A'^3A^{(3)} - 12A^3A'A''A^{(3)} + 8A^3A'^2A^{(4)} + 2A^4A'A^{(5)}\Big)...$$

"Linear" approximation:

$$D(x) \simeq \; 1 - \frac{\epsilon}{3} A'^2 + \frac{\epsilon^2}{5} A'^4 - ... + \frac{(-\epsilon)^j}{2j+1} A'^{2j} + ... = \frac{\arctan(\sqrt{\epsilon}A')}{\sqrt{\epsilon}A'}$$

3D symmetric channels : $\quad D(x) \simeq \dfrac{1}{\sqrt{1 + \epsilon R'^2(x)}}\,; \qquad R(x)$ is the radius

$\sqrt{\epsilon}$ as a scaling parameter of the transverse lengths

If we rescale $\sqrt{\epsilon}y \to y$, $\sqrt{\epsilon}A(x) \to A(x)$ and $\rho \to \sqrt{\epsilon}\rho$ the diffusion becomes isotropic:

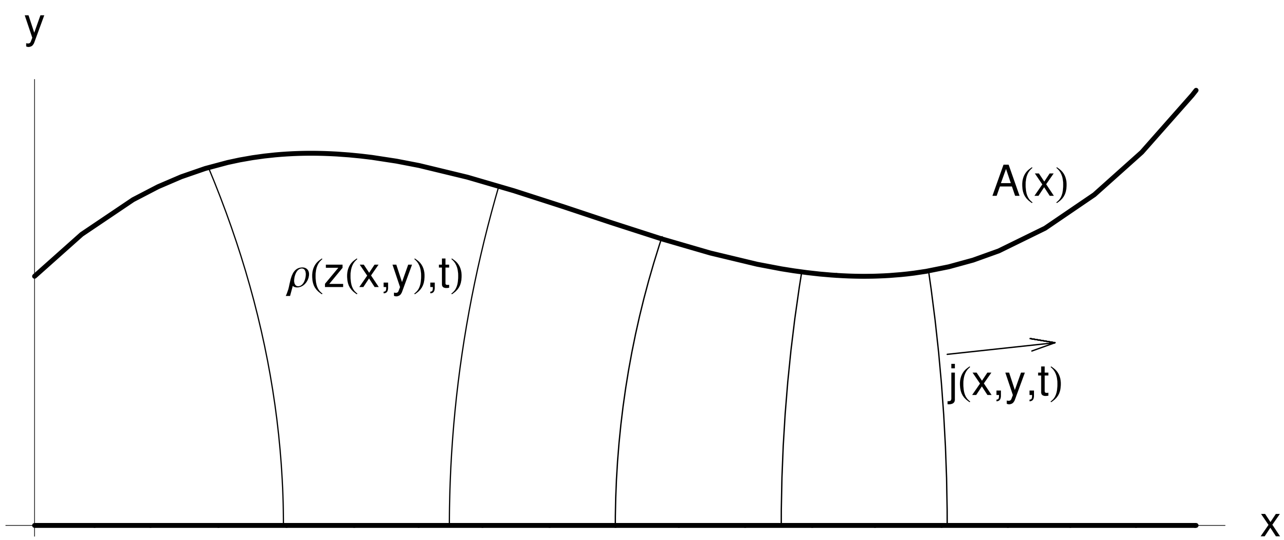
$$\frac{\partial}{\partial t}\frac{\rho(x,y,t)}{\sqrt{\epsilon}} = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial(\sqrt{\epsilon}y)^2}\right)\frac{\rho(x,y,t)}{\sqrt{\epsilon}} \;;$$

the upper boundary condition:

$$\frac{\partial\rho(x,y,t)}{\sqrt{\epsilon}\;\partial(\sqrt{\epsilon}y)} = \sqrt{\epsilon}A'(x)\frac{\partial\rho(x,y,t)}{\sqrt{\epsilon}\;\;\partial x}\bigg|_{\sqrt{\epsilon}y=\sqrt{\epsilon}A(x)} \;.$$

$\Rightarrow$ a narrow channel with isotropic diffusion is equivalent to a wide domain with $D_y \gg D_x$.

Variational approach



Q: Can we express the 2D density $\rho(x, y, t)$ as a function of only one spatial (curvilinear) variable $z = z(x, y)$?

Variational mapping: we start from the functional $F[\rho,\bar\rho]$

$$F=\int_{t_0}^{t_1}dt\int_{x_L}^{x_R}dx\int_0^{A(x)}dy\Big(\frac{1}{2}\Big(\dot\rho\bar\rho-\dot{\bar\rho}\rho\Big)+\partial_x\bar\rho\;\partial_x\rho+\frac{1}{\epsilon}\partial_y\bar\rho\;\partial_y\rho\Big)$$

Stationary condition $\delta F=0$ gives the diffusion and "*anti* diffusion" equation for the density $\rho=\rho(x,y,t)$ and its complementary $\bar\rho=\bar\rho(x,y,t)$:

$$\dot\rho=\partial_x^2\rho+\frac{1}{\epsilon}\partial_y^2\rho \quad ; \qquad -\dot{\bar\rho}=\partial_x^2\bar\rho+\frac{1}{\epsilon}\partial_y^2\bar\rho$$

Next step: switching from (x,y) to (z,y) in F

$$F=\int_{t_0}^{t_1}dt\int_{z_L}^{z_R}dz\int_0^{A(x_z)}dy\frac{\partial x}{\partial z}\Big[\frac{1}{2}\Big(\dot\rho\bar\rho-\dot{\bar\rho}\rho\Big)+\Big(\Big(\frac{\partial z}{\partial x}\Big)^2+\frac{1}{\epsilon}\Big(\frac{\partial z}{\partial y}\Big)^2\Big)\partial_z\bar\rho\,\partial_z\rho\Big]$$

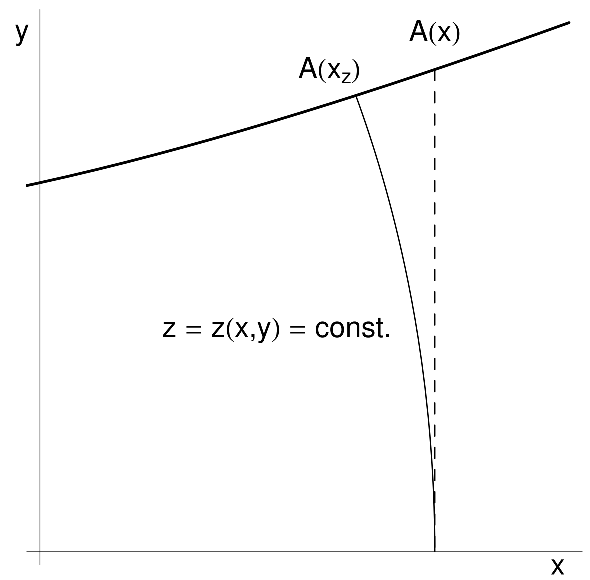
$x=x(z,y)$ is inverse to $z=z(x,y)$ and $x_z=x\big(z,A(x_z)\big)$.

Integration over y – along constant $z = z(x,y)$:

$$F_1[\rho(z,t), \bar{\rho}(z,t)] = \int_{t_0}^{t_1} dt \int_{z_L}^{z_R} dz \left[\frac{1}{2}\alpha(z)\Big(\dot{\rho}\bar{\rho} - \dot{\bar{\rho}}\rho\Big) + \kappa(z)\ \partial_z\bar{\rho}\ \partial_z\rho\right] \ ;$$

$$\alpha(z) = \int_0^{A(x_z)} dy \frac{\partial x}{\partial z} \qquad \text{and}$$

$$\kappa(z) = \int_0^{A(x_z)} dy \Big(\frac{\partial x}{\partial z}\Big)^{-1}\left(1 + \frac{1}{\epsilon}\Big(\frac{\partial x}{\partial y}\Big)^2\right) \ .$$



Stationary condition $\delta F_1[\rho, \bar{\rho}] = 0$ gives
the mapped equation:

$$\frac{\partial \rho}{\partial t} = \frac{1}{\alpha(z)}\frac{\partial}{\partial z}\kappa(z)\frac{\partial}{\partial z}\rho \quad ; \qquad -\frac{\partial \bar{\rho}}{\partial t} = \frac{1}{\alpha(z)}\frac{\partial}{\partial z}\kappa(z)\frac{\partial}{\partial z}\bar{\rho}$$

A problem: there is no condition for the transformation $z = z(x, y)$

– at the stationary $\rho, \bar{\rho}$, $F[\rho, \bar{\rho}] = 0$ for **any** $z = z(x, y)$.

Simple Ansatz:

$$z = z(x, y) = \sum_{j=0}^{\infty} \epsilon^j y^{2j} z_j(x)$$

– the boundary conditions for $\rho\big(z(x, y), t\big)$ have to be satisfied

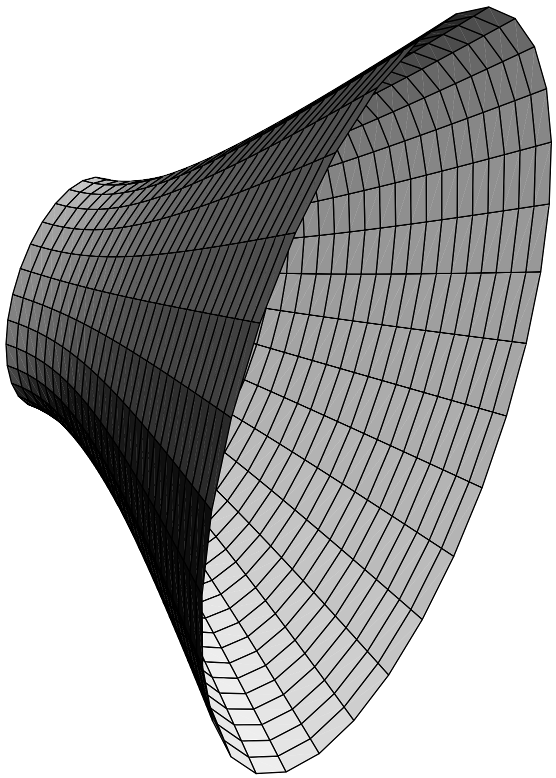
$$\frac{\partial \rho}{\partial z} \frac{\partial z}{\partial y} = 0 \Big|_{y=0} \quad ; \quad \frac{1}{\epsilon} \frac{\partial \rho}{\partial z} \frac{\partial z}{\partial y} = A'(x) \frac{\partial \rho}{\partial z} \frac{\partial z}{\partial x} \Big|_{y=A(x)} \ ;$$

hence

$$z_j(x) = \frac{1}{2j} \frac{A'(x)}{A(x)} \ z'_{j-1}(x) \ ;$$

$z_0(x)$ can be chosen to make the Ansatz summable.

Test example - hyperboloidal cone



Oblate spheroidal coordinates:

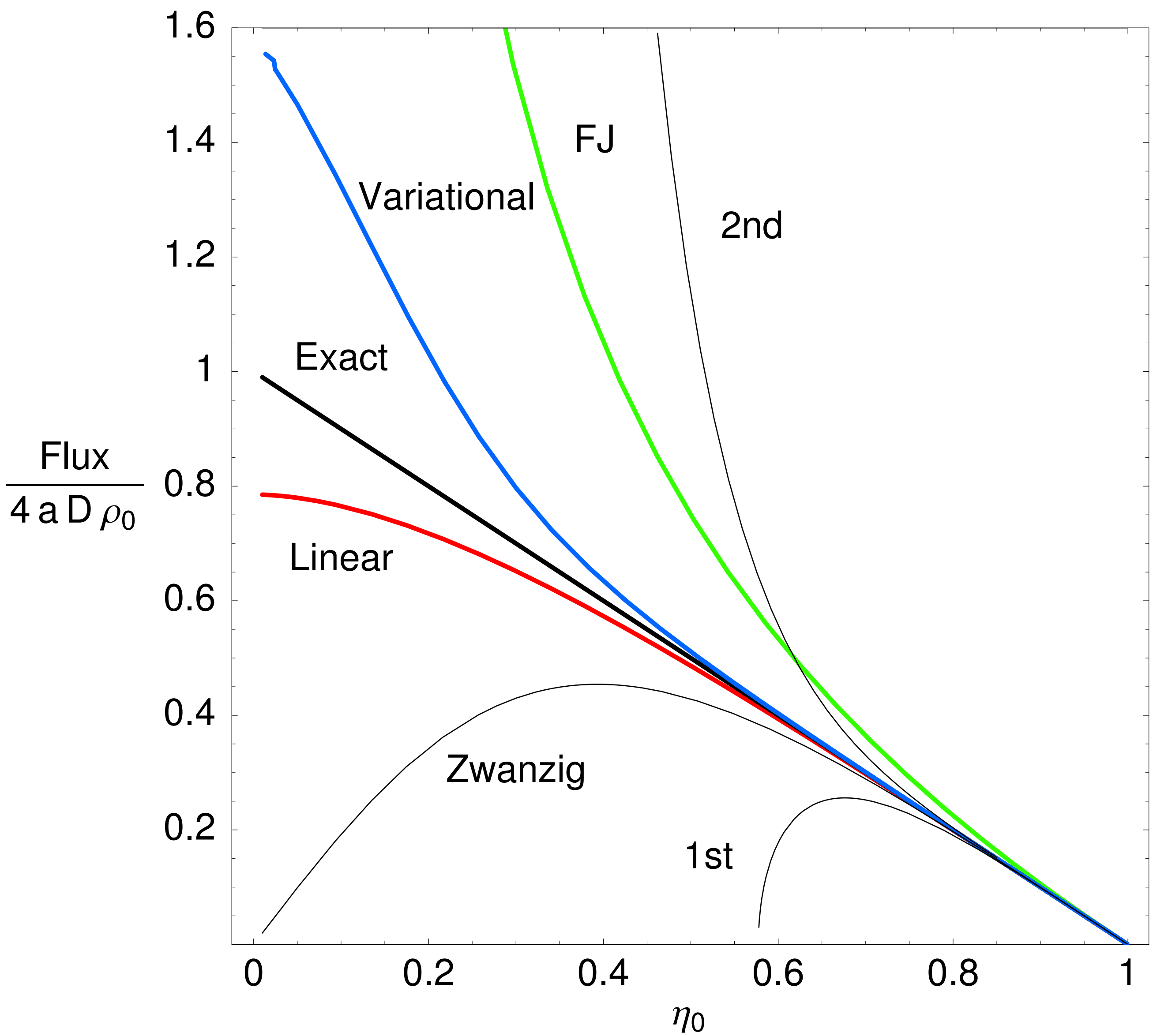
$$x = a\xi\eta, \qquad r^2 = a^2(1+\xi^2)(1-\eta^2)$$

ξ – longitudinal coordinate; $\xi > 0$
η – curved transverse coordinate,
hard walls at $\eta = \eta_0$; $0 < \eta_0 < 1$
the points $\eta_0 < \eta < 1$ are inside the cone

Boundary conditions:

- $\xi = 0$ absorbing boundary; $\rho(0, \eta) = 0$
- in infinity, $\rho(\xi \to \infty, \eta) \to \rho_0 = const.$

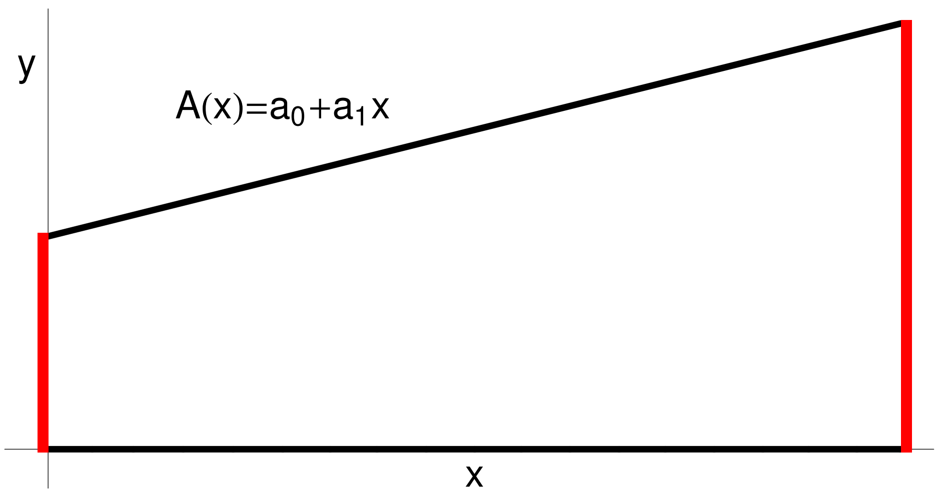
Q: What is the stationary flux J through the bottleneck $(x = \xi = 0)$?



1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
Flux / 4 a D ρ_0
0
0.2
0.4
0.6
0.8
1
η_0
FJ
Variational
2nd
Exact
Linear
Zwanzig
1st

… several questions:

- how to find the optimal transformation $z = z(x, y)$?
- how reliable is the "linear" formula for $D(x)$?
- can we sum more terms in the ϵ- expansion of $D(x)$?



A. M. Berezhkovskij, M. A. Pustovoit and S. M. Bezrukov: J Chem. Phys. **126**, 134706 (2007)

Stationary curvilinear coordinates

The mapped equation : $$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x} A(x) D(x) \frac{\partial}{\partial x} \frac{p(x,t)}{A(x)}$$

Its stationary solution : $$\frac{p(x)}{A(x)} = \rho_0 - J \int \frac{dx'}{A(x')D(x')}$$

$D(x)$ is fixed by using $\hat{Z}(x, \partial_x)$ and $\hat{\omega}(x, y, \partial_x)$ is known, hence

$$\rho(x,y) = \hat{\omega}(x,y,\partial_x) \frac{p(x)}{A(x)} = \rho_0 + J \sum_{j=0}^{\infty} \sum_{k=0}^{j} \epsilon^j y^{2k} z_{j,k}(x) = \rho_0 + J z(x,y) \; ;$$

$$z_{0,0}(x) = \int \frac{dx}{A(x)} \,, \quad z_{1,0}(x) = \frac{1}{3} \int \frac{A'^2}{A} dx - \frac{A'}{6} \,, \quad z_{1,1}(x) = \frac{A'}{2A^2} \,, \ldots$$

Correspondence to electrostatics

Conversely, the stationary ρ solves $\Delta\rho(x,y) = 0$ plus Neumann BC at $y = 0, A(x)$, so $D(x)$ can be calculated directly from

$$-J = A(x)D(x)\frac{\partial}{\partial x}\left[\frac{1}{A(x)}\int_0^{A(x)} \rho(x,y)dy\right]$$

for exactly solvable geometries in electrostatics.

Q: Why do we need $D(x)$ if we have already the 2D solution $\rho(x,y)$?

A: Originally, we intended to use the mapped equation for description of **non stationary processes**.

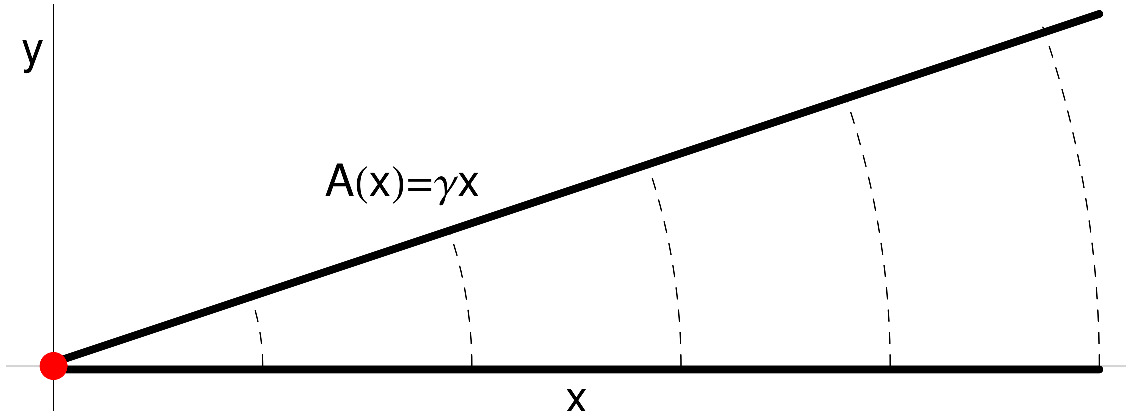
- the simplified mapped equation (with $D(x)$) is capable to describe only quasi-stationary processes.

Linear cone:

single charge at $(0,0)$

$$\rho(x,y) = \rho_0 + c\ln r$$

where $r = \sqrt{x^2+y^2}$.



Fixing $c:\quad J = -\int_0^{A(x)} \partial_x \rho(x,y)dy \quad \Rightarrow \quad \rho(x,y) = \rho_0 - \frac{J\ln r}{\arctan\gamma}$

$$D(x) = -\frac{J}{\gamma x}\left(\frac{\partial}{\partial x}\left[\frac{1}{\gamma x}\int_0^{\gamma x}\rho(x,y)dy\right]\right)^{-1} = \frac{\arctan\gamma}{\gamma}$$

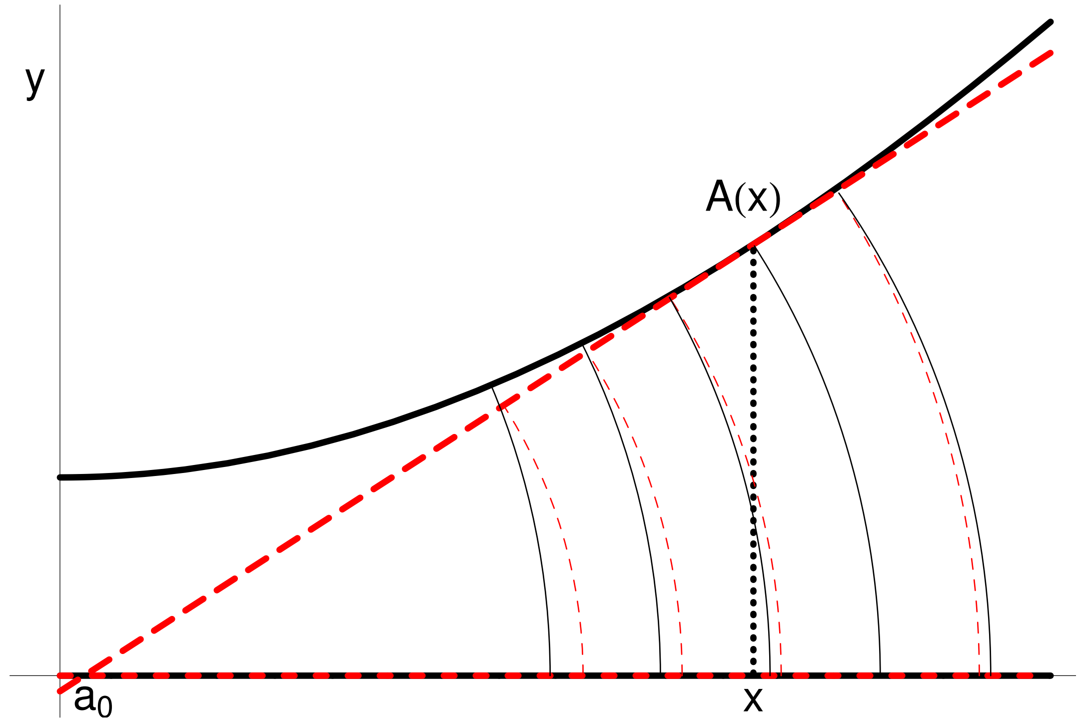
$r = \sqrt{x^2+y^2}$ – correct curvilinear coordinate for the variational mapping.

Linear approximation:

$A(x)$ is approximated by its tangent at x;

$$a_0 = x - \frac{A(x)}{A'(x)}$$

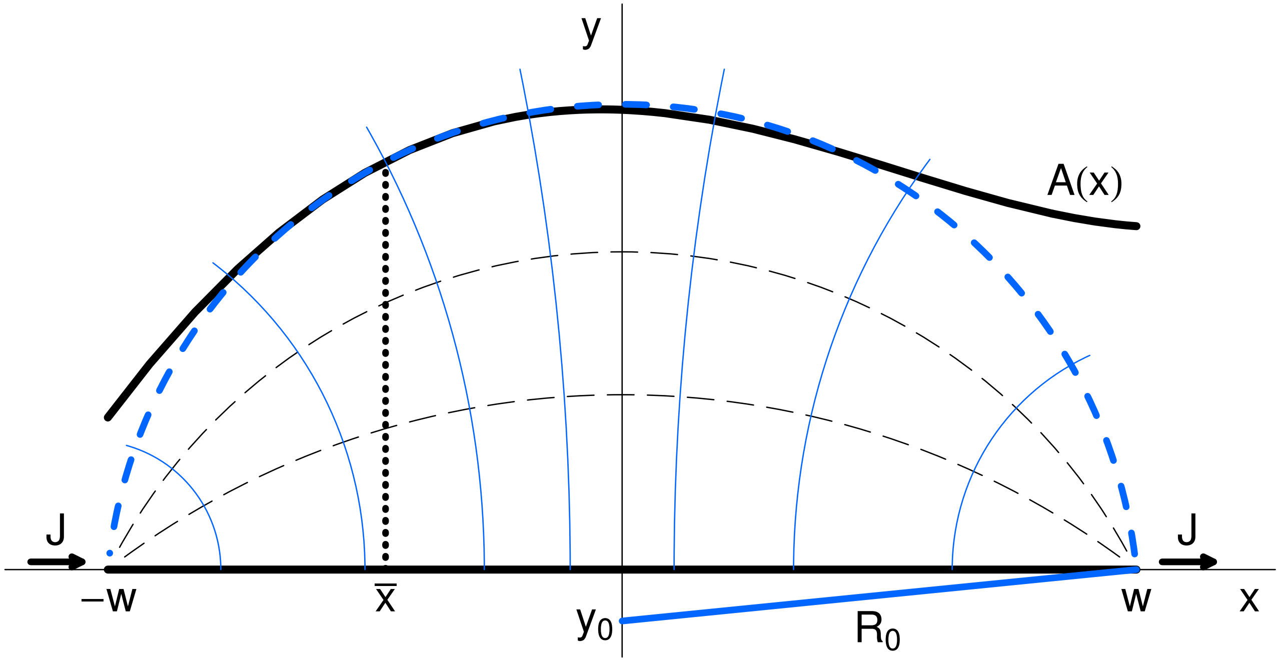
In the linear cone,



$$\rho(x,y) = \rho_0 - \frac{J}{2\arctan\gamma}\ln\left[(x-a_0)^2 + y^2\right]\ ; \qquad \gamma = A'(x) \text{ is constant}$$

$$D(x) = \frac{-J}{\gamma(x-a_0)}\left(\frac{\partial}{\partial x}\left[\frac{1}{\gamma(x-a_0)}\int_0^{\gamma(x-a_0)} \rho(x,y)dy\right]\right)^{-1} = \frac{\arctan A'(x)}{A'(x)}$$

Circular approximation:



$A(x)$ is approximated by a circle, given by 3 parameters: radius R_0, and the shifts x_0, y_0;

- the circle fits $A(x)$, $A'(x)$ and $A''(x)$ at $x = \bar{x}$.

$$\rho(x, y) = \rho_0 - \frac{J}{2 \arctan[-w/y_0]} \ln \frac{(w + x - x_0)^2 + y^2}{(w - x + x_0)^2 + y^2} \, ,$$

where $w = \sqrt{R_0^2 - y_0^2}$ and arctan of real argument $\in (0, \pi)$.

$$D(x) = \frac{AA''}{A'(1+A'^2+AA'')\arctan(A')/\arctan(\gamma) + AA'' - A'^2(1+A'^2)}\,,$$

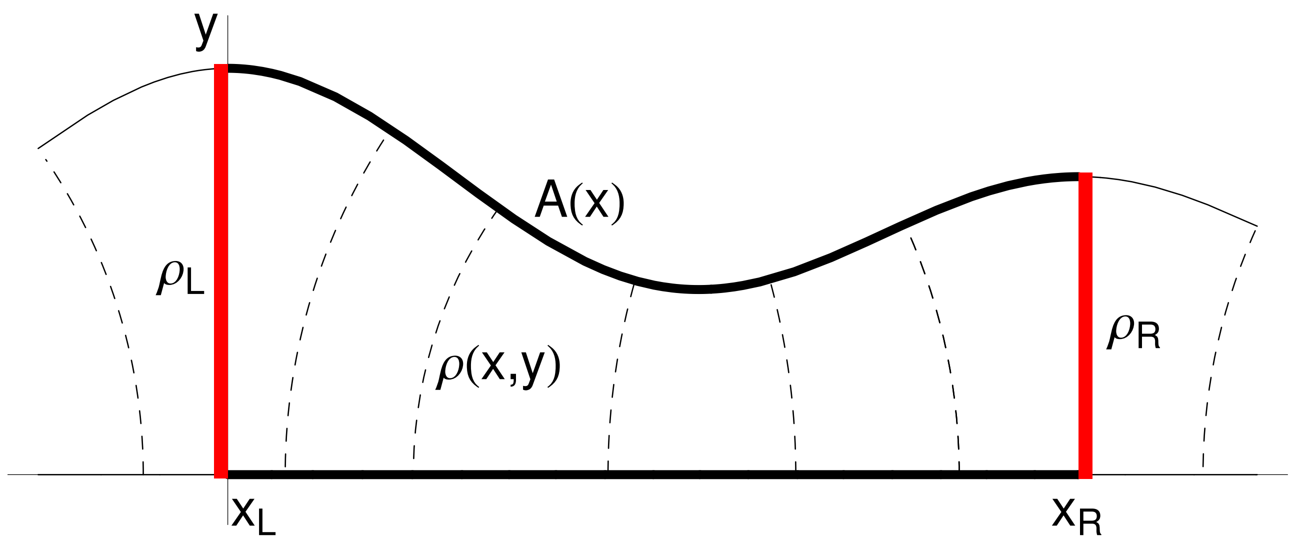
$$\text{where} \qquad \gamma = \frac{\sqrt{(1+A'^2)^3 - (1+A'^2+AA'')^2}}{1+A'^2+AA''}$$

If A is rescaled by $\sqrt{\epsilon}$, its Taylor expansion is

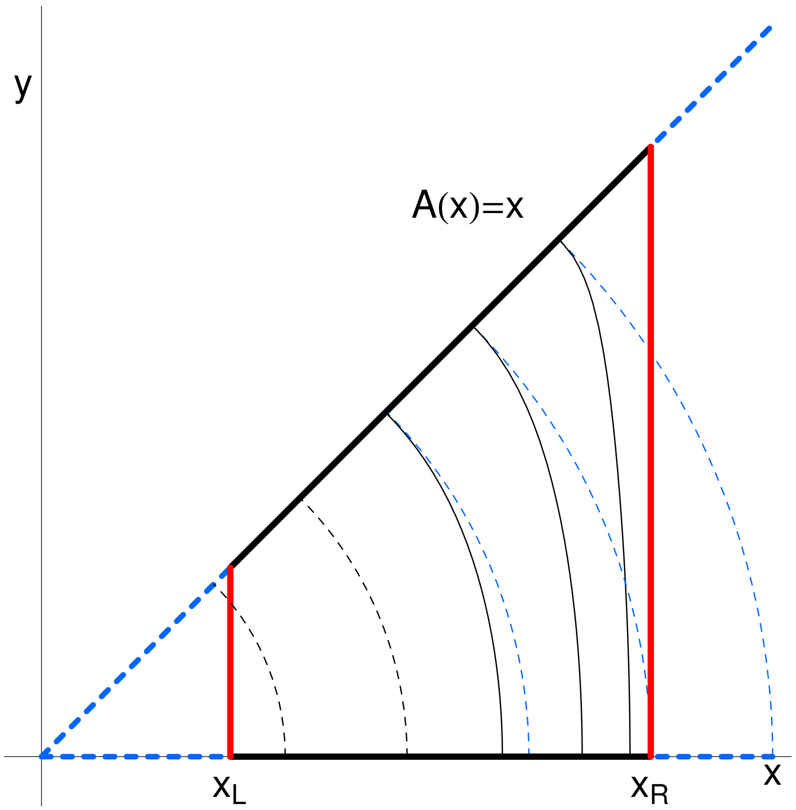
$$D(x) = 1 - \frac{\epsilon}{3}A'^2 + \frac{\epsilon^2}{45}A'^2(9A'^2 + AA'') - \frac{\epsilon^3}{945}A'^2(135A'^4 + 45AA'^2A'' + 5A^2A''^2) + \ldots$$

Finite channels

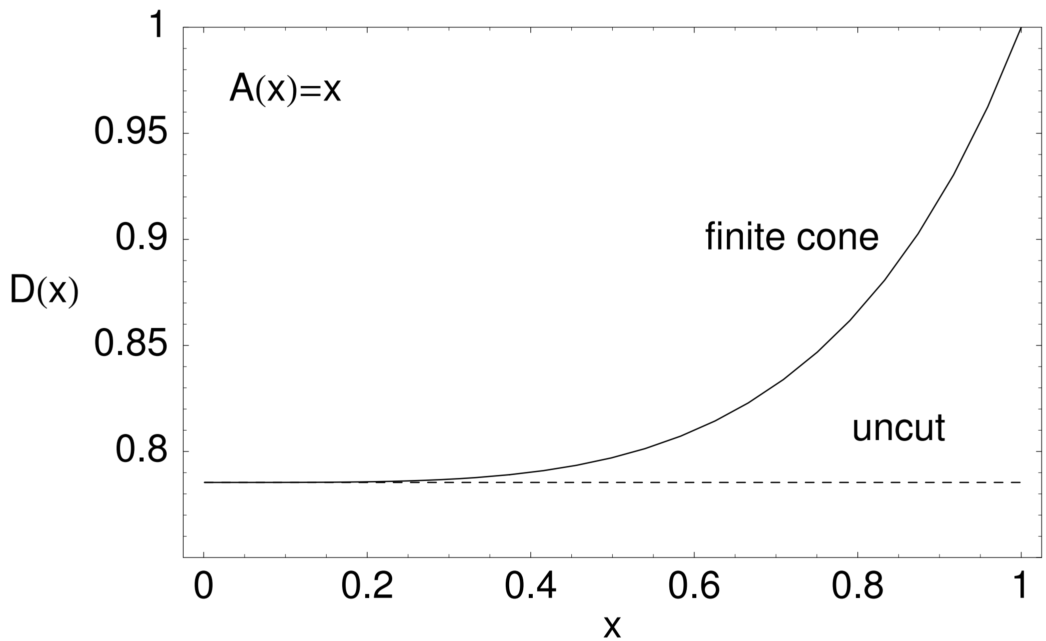
- the mapping procedure supposes that **the function $A(x)$ is analytic**
- the mapping generates a unique stationary curvilinear system
- if the function $A(x)$ defined for $x \in (x_L, x_R)$ is extended by its mirrors $A(x_{L,R} + x) = A(x_{L,R} - x)$ and it remains analytic, the mapping works



Finite linear cone



- calculated by using electrostatics for $x_L = 0$, $x_R = 1$



Hierarchy of approximations of the mapping

- **Zwanzig-Mori:** keeps all information; the transients are hidden in the memory
- **non stationary mapping:** projects out the transients, the mapped process is again Markovian, governed by the generalized **FJ equation** modified by a **correction operator** $1 - \hat{Z}(x, \partial_x)$
- **stationary mapping:** fixes a unique curvilinear coordinate system; **the operator** $1 - \hat{Z}(x, \partial_x)$ becomes **a function** $D(x)$.
- **next approximations** of $D(x)$. The exact stationary function is replaced by a function $D(x)$ corresponding to **some exactly solvable model**, which approximates the true boundary.

Can be this mapping extended to other dynamics?

forced diffusion; diffusion in an external field . . . is OK

ballistic motion - ?

quantum mechanics - ?

One has to resolve ...

... what are the transients?

... what is the small parameter ϵ?

... what is an equivalent of the Fick-Jacobs equation?

... what plays the role of the equilibrium in non-dissipative processes?

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