PROJECTING DIFFUSION ALONG THE NORMAL BUNDLE OF A PLANE CURVE

CARLOS VALERO VALDES
DEPARTAMENTO DE MATEMATICAS APLICADAS Y SISTEMAS
UNIVERSIDAD AUTONOMA METROPOLITANA-CUAJIMALPA
MEXICO, D.F 01120, MÉXICO

RAFAEL HERRERA GUZMAN
CENTRO DE INVESTIGACION EN MATEMATICAS (CIMAT)
GUANAJUATO, GTO
MEXICO.

Abstract. The purpose of this paper is to provide new formulas for the effective diffusion coefficient of a generalized Fick-Jacob’s equation obtained by projecting the two-dimensional diffusion equation along the normal directions of an arbitrary curve on the plane.

1. Introduction

The problem of understanding spatially constrained diffusion in quasi-one dimensional systems plays a fundamental role in diverse scientific areas such as biology (e.g. channels in biological systems), chemistry (e.g. pores in zeolites) and nanotechnology (e.g. carbon nano-tubes). Solving the diffusion equation for general channel-like constraining geometries represents a very difficult task. One approach to overcome this situation consists in reducing the degrees of freedom of the problem by considering only the main direction of transport. More concretely, consider a channel-like geometry bounded from below and above by two functions $y = y_1(x)$ and $y = y_2(x)$ (see Figure 1.1), and a concentration density function $P = P(x, y, t)$ satisfying the diffusion equation

$$ \frac{\partial P}{\partial t} (x, y, t) = D_0 \left( \frac{\partial^2 P}{\partial x^2} (x, y, t) + \frac{\partial^2 P}{\partial y^2} (x, y, t) \right) $$

and having no flow across the channel’s walls. If we integrate $P$ with respect to the $y$-coordinate we obtain an effective density function

$$ p(x, t) = \int_{y_1(x)}^{y_2(x)} P(x, y, t) dy, $$

whose values represent the total concentration density along vertical cross sections of the channel. The dynamics of $p$ can be modeled in an approximate manner by a generalized Fick-Jacob’s equation

$$ \frac{\partial p}{\partial t} (x, t) = \frac{\partial}{\partial x} \left( D(x) w(x) \frac{\partial}{\partial x} \left( \frac{p(x, t)}{w(x)} \right) \right), $$

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Figure 1.1. Channel geometry defined as the set for point \((x, y)\) such that \(y_1(x) \leq y \leq y_2(x)\).

where the function \(D = D(x)\) is known as the effective diffusion coefficient and \(w(x) = y_2(x) - y_1(x)\) is the channel’s width. The precision of the approximation that the generalized Fick-Jacob’s provide compared to the true time evolution of \(p\) depends on an adequate estimation of the effective diffusion coefficient. The simplest estimate for \(D\) is the one given by \(D(x) = D_0\), which arises from the assumption that the density \(P\) stabilizes infinitely fast in the transversal direction (i.e \(P\) is independent of \(y\)). Better estimations of \(D\) must account for the fact that in reality the transversal diffusion rate is finite. Work in this direction was carried out by Zwanzig in [9] where he obtained the formula

\[
D(x) = D_0 \left(1 + \frac{w'(x)^2}{12}\right) \quad \text{where} \quad w'(x) = \frac{dw}{dx}(x),
\]

which then Bradley generalized in [1] to

\[
D(x) = D_0 \left(1 + \frac{y_0'(x)^2 + w'(x)^2}{12}\right) \quad \text{where} \quad y_0(x) = \frac{y_1(x) + y_2(x)}{2},
\]

to deal with non-symmetric channels (i.e \(y_0 \neq 0\)). Reguera and Rubí in [7] also proposed an improvement of Zwanzig’s formula, given by

\[
D(x) = D_0 \left(\frac{1}{1 + w'(x)^2/4}\right)^{1/3}.
\]

Later on Kalinay & Percus developed in [5] a systematic procedure to obtain increasingly better formulas to \(D\), and which they used to derived the formula

\[
D(x) = D_0 \left(\frac{\arctan(w'(x)/2)}{w'(x)/2}\right)
\]

under the assumption that \(y_1(x) = 0\). This formula was then extended, dropping the assumption \(y_1(x) = 0\), by L. Dagdug & I. Pineda in [2] to obtain

\[
D(x) = D_0 \left(\frac{\arctan(y_0'(x) + w'(x)/2) - \arctan(y_0'(x) - w'(x)/2)}{w'(x)/2}\right).
\]
The results described above deal with the “projection” of a two dimensional density function onto a the $x$-coordinate of the standard coordinates $(x, y)$ on the plane. As an example where these coordinates are not the best choice consider a channel-like geometry as the one depicted in Figure 1.2 in which it is more natural to use polar coordinates. The use of coordinate functions that follow in a “natural manner” the geometry of the channel can help in the calculation of effective diffusion coefficient (see [4]). Furthermore, to study quasi-one dimensional diffusion on a curved surface (e.g. the surface of a cell) one is forced from the beginning to consider more general coordinate systems than the standard $(x,y)$ system in the plane.

The purpose of this paper is to generalize the work described above by deriving formulas for the effective diffusion coefficient (in the infinite and finite transversal diffusion rate cases) for channels defined on a system of coordinates $u,v$ constructed as follows. For an arbitrary curve in the plane (which we will refer as the base curve) we will let $u$ be base curve’s arc-length parameter with respect to a fixed reference point, and we will let $v$ be the normal distance to the base curve (see Figure 1.3). As before, we can then construct channels over the base curve by using a pair of functions $v_1 = v_1(u)$ and $v_2 = v_2(u)$ (see Figure 3.1). In a similar way as in the case of rectangular coordinates, from the density function $P$ we can construct an effective density function $p = p(u,t)$ whose evolution can be modeled (in an approximate way) by a generalized Fick-Jacob’s equation of the form

$$\frac{\partial p}{\partial t} (u,t) = \frac{\partial}{\partial u} \left( D(u) \sigma(u) \frac{\partial}{\partial u} \left( \frac{p(u,t)}{\sigma(u)} \right) \right).$$
In the above formula $D = D(u)$ stands for the effective diffusion coefficient, and the function $\sigma$ is given by

$$\sigma(u) = \frac{dA}{du}(u),$$

where $A(u)$ defined as the area of the channel from the transversal section at the reference point to the transversal section over the point on the base curve with coordinate $u$. In the case when the base curve in the $x$-axis the function $\sigma$ coincides with the channel’s width function.

The outline of our article is as follows:

- In section 2 we will show that if the concentration density in the plane satisfies the continuity equation (given by formula 2.1) then the corresponding effective density also obeys a continuity equation (see formula 2.3). This last equation, which we will refer as the effective continuity equation, will serve as the basis for the work that follows in the rest of the article.
- In section 3 we will derive the formula for the effective diffusion coefficient corresponding to the infinite transversal diffusion rate (see formula 3.6). The obtained formula generalizes the standard Fick-Jacob’s equation in the sense it is a particular case of ours for a base curve that has zero curvature (i.e it is a straight line). We end the section by applying our formulathed to derive some interesting physical properties of symmetric channels of constant width.
- In sub-section 4.1 we derive our first formula for the effective diffusion coefficient corresponding to a finite transversal diffusion rate. Our formula in this case involves tangential information (i.e derivatives) of the curves forming the upper and lower boundaries of the channel. We show that the obtained formula generalizes the results of L. Dagdug and I. Pineda [2]. Again, their formula can be recovered from ours as the case when the base curve has zero curvature. It is interesting to observe that in the zero curvature case the effective diffusion coefficient is always less than or
equal to the diffusion coefficient \( D_0 \) for the corresponding the 2-dimensional diffusion equation. In contrast, in the general case of projecting onto an arbitrary curve the effective diffusion coefficient can be less than, greater than or equal to \( D_0 \).

- In sub-section 4.2 we derive our second formula for the effective diffusion coefficient corresponding to a finite transversal diffusion rate. In this case our formula involves both tangential and curvature information of the curves forming of the upper and lower boundaries of the channel. We show that for symmetric channels of constant width the infinite transversal diffusion rate case coincides with current case. This confirms our intuition that the choice of an appropriate coordinate systems simplifies the computation of the effective diffusion coefficient.

We will use the language of the differential geometry of planar curves to write down the formula for \( D \) in a coordinate-free manner. Furthermore, we use complex analysis to provide a more compact expression for \( D \) than would otherwise be obtained by using only real analysis. In particular, our use of the complex logarithm function will help us unify different cases which otherwise would appear to be unrelated.

2. The effective continuity equation on the plane

We will identify 2-dimensional space \( \mathbb{R}^2 \) with the complex plane \( \mathbb{C} \) by means of the correspondence: \((x, y) \leftrightarrow z = x + iy\). To distinguish the dot product in \( \mathbb{R}^2 \) from the complex product in \( \mathbb{C} \) we will use the symbol \(<,>\) for the former and simple juxtaposition for the latter.

We are interested in describing transport processes on a region \( \Omega \) of the plane which are modeled by the continuity equation

\[
\frac{\partial P}{\partial t} + \text{div}(J) = 0,
\]

where \( P = P(z, t) \) is a real valued density function and \( J = J(z, t) \) is its corresponding complex valued flux. We will apply a dimensionality reduction technique to this equation as follows. Let us assume that \( \Omega \) is parametrized by a smooth map \( \varphi : [u_1, u_2] \times [a, b] \rightarrow \Omega \), and consider the following subsets of \( \Omega \) (see Figure 2.1):

\[
\Omega_u = \varphi([u_1, u] \times [a, b]),
\]

\[
\Omega^a = \{ \varphi(u, a)|u_1 \leq u \leq u_2 \},
\]

\[
\Omega^b = \{ \varphi(u, b)|u_1 \leq u \leq u_2 \}.
\]

We will refer to \( \Omega^a \) and \( \Omega^b \) as lower and upper walls of \( \Omega \). The total concentration of \( P \) in the region \( \Omega_u \) is given by

\[
C(u, t) = \int_a^b \int_{u_1}^u P(\varphi(s, v), t) \det(\varphi'(s, v))dvds,
\]

where \( \varphi' \) is the Jacobian matrix of \( \varphi \). The effective density \( p \) associated to \( P \) is defined as

\[
p(u, t) = \frac{dC}{du}(u, t) = \int_a^b P(\varphi(u, v), t) \det(\varphi'(u, v))dv,
\]
and the corresponding effective flux $j$ by

$$j(u,t) = \int_a^b \left< i J(\varphi(u,v), t), \frac{\partial \varphi}{\partial v}(u,v) \right> dv,$$

The quantity $p(u,t)$ measures the density concentration at time $t$ along the cross section parametrized by $v \mapsto \varphi(u,v)$, and $j(u,t)$ measures the flux density along the same cross section. If we assume that there is no flux of $P$ across the upper and lower walls of $\Omega$ then the two-dimensional continuity equation (2.1) implies the effective continuity equation

$$\frac{\partial p}{\partial t}(u,t) + \frac{\partial j}{\partial u}(u,t) = 0.$$

If we impose Fick’s law

$$J = -D_0 \nabla P,$$

for a constant diffusion coefficient $D_0$, the two-dimensional continuity equation becomes the diffusion equation

$$\frac{\partial P}{\partial t} = D_0 \Delta P.$$

In this case, the effective flux becomes

$$j(u,t) = -D_0 \int_a^b \left< i \nabla P(\varphi(u,v), t), \frac{\partial \varphi}{\partial v}(u,v) \right> dv.$$

3. A GENERALIZED FICK-JACOB’S EQUATION ON THE NORMAL BUNDLE OF A PLANE CURVE: INFINITE TRANSVERSAL DIFFUSION RATE CASE

Consider a curve $\alpha : [u_1, u_2] \rightarrow \mathbb{C}$ parametrized by the arc-length parameter $u$. Under this assumption the vectors

$$T = \frac{\partial \alpha}{\partial u} \text{ and } N = i \frac{\partial \alpha}{\partial u}$$
Figure 3.1. Channel over normal bundle of a curve

are the unit tangent and unit normal vectors of \( \alpha \). We will consider a region \( \Omega \) parametrized by the map \( \varphi : [u_1, u_2] \times [-1, 1] \rightarrow \mathbb{R}^2 \) given by

\[
\varphi(u, v) = \alpha(u) + s(u, v)N(u),
\]

where

\[
s(u, v) = v_0(u) + vw(u)/2,
\]

for given functions \( v_0, w : [u_1, u_2] \rightarrow \mathbb{R} \). We will refer to \( v_0 \) as the middle curve function and to \( w \) as the width function. The lower and upper curves \( \alpha_1 \) and \( \alpha_2 \) are then given by

\[
\begin{align*}
\alpha_1(u) &= \varphi(u, -1) = \alpha(u) + (v_0(u) - w(u)/2)N, \\
\alpha_2(u) &= \varphi(u, 1) = \alpha(u) + (v_0(u) + w(u)/2)N,
\end{align*}
\]

and we define the middle curve \( \alpha_0 \) by

\[\alpha_0(u) = \varphi(u, 0) = \alpha(u) + v_0(u)N.\]

Observe that in general \( \alpha_0 \) and \( \alpha \) do not coincide (see Figure 3.1). By using the formulas (see Appendix 1)

\[
\frac{dT}{du} = kN \quad \text{and} \quad \frac{dN}{du} = -kT,
\]

where \( k \) is the curvature function of \( \alpha \), we obtain the equations

\[
\begin{align*}
\frac{\partial \varphi}{\partial u} &= (1 - sk)T + \frac{\partial s}{\partial u}N, \\
\frac{\partial \varphi}{\partial v} &= (w/2)N,
\end{align*}
\]
In this case, the effective density (2.2) becomes

\[ p = \int_{-1}^{1} P(1 - sk)(w/2) dv. \]

To compute the effective flux (2.4) observe that

\[ \frac{\partial P}{\partial u} = \left( \nabla P, \left( \frac{\partial \varphi}{\partial u} \right) \right) = (1 - sk) \left( \nabla P, T \right) + \frac{\partial s}{\partial u} \left( \nabla P, N \right) \]

and

\[ \frac{\partial P}{\partial v} = \left( \nabla P, \left( \frac{\partial \varphi}{\partial v} \right) \right) = \left( \frac{w}{2} \right) \left( \nabla P, N \right). \]

From the above formulas and the definition of \( j \) we obtain

\[ j = -D_0 \int_{-1}^{1} \left( \frac{w}{2} \right) < \nabla P, T > dv \]

The hypothesis of an infinite diffusion rate along the \( v \)-variable means that \( P \) is independent of that variable, and hence we obtain

\[ p(u, t) = \sigma(u) P(u, t), \]

\[ j(u, t) = -D_0 \gamma(u) \frac{\partial P}{\partial u}(u, t), \]

where

\[ \sigma(u) = \frac{1}{2} \int_{-1}^{1} (1 - s(u, v)k(u))w(u)dv, \]

\[ \gamma(u) = \frac{1}{2} \int_{-1}^{1} (1 - s(u, v)k(u))^{-1}w(u)dv. \]

From the results above, we conclude that the effective continuity equation (2.3) becomes the following generalized Fick-Jacob’s equation

\[ \frac{\partial p}{\partial t}(u, t) = \frac{\partial}{\partial u} \left( D(\sigma) \frac{\partial}{\partial u} \left( \frac{p(u, t)}{\sigma(u)} \right) \right), \]

where

\[ D = \left( \frac{D_0}{k w} \right) \left( \frac{1}{1 - kv_0} \right) \log \left( \frac{1 - k(v_0 - w/2)}{1 - k(v_0 + w/2)} \right), \]

\[ \sigma = w(1 - kv_0). \]

We will refer to \( D \) as the effective diffusion coefficient. Observe that \( \sigma \) in equation (3.5) plays the role of the width in the classical Fick-Jacob’s equation. The function \( \sigma \) is an area density since the area of the region \( \Omega_u = \varphi([u_1, u]) \) is given by

\[ A(u) = \int_{u_1}^{u_2} \sigma(a) da. \]
For a symmetric channel \((v_0 = 0)\) we have that \(\sigma = w\), i.e. we recover the width function, and

\[(3.7) \quad D = \frac{D_0}{kw} \log \left( \frac{1 + kw/2}{1 - kw/2} \right).\]

If we consider \(D\) as a function of \(w\) and \(k\), its level sets are the hyperbolas \(kw = \text{constant}\) and its gradient lines are the hyperbolas \(w^2 - k^2 = \text{constant}\) (see Figure 3.2). It is easily seen that

\[
\lim_{kw \to 0} D(k, w) = D_0, \\
\lim_{kw \to 2} D(k, w) = \infty.
\]

Thus we have the following observations about symmetric channels of constant width.

1. The value of the effective diffusion coefficient remains constant if we keep \(w\) and \(k\) inversely proportional. In particular, if we increase the curvature of a channel (e.g. by bending it) then we must reduce its width to keep the effective diffusion constant.

2. The effective diffusion coefficient coincides with the diffusion coefficient of the non-reduced diffusion equation when either the curve has zero width and arbitrary curvature function, or the base curve is a straight line (i.e. \(k = 0\)) with arbitrary width function.

3. The limit \(\lim_{kw \to 2} D(k, w) = \infty\) means the channel is such that its upper or lower walls contain focal points of the base curve. This situation is a consequence of the degeneracy of the coordinate system induced by the normal lines of the base curve. To avoid this complication the upper and lower walls of the channel must stay close to the base curve, assumption which is consistent with the fact that we are dealing with narrow channels.

4. Observe that for symmetric channels of constant width the effective diffusion coefficient is always larger than \(D_0\). For example, if we take a straight cylindrical tube and bend it (so that its walls remain at a constant distance from the base curve) then the effective diffusion increases.

Remark. As explained in point 2 above, the effective diffusion coefficient can become infinite due to the existence of focal points of the base curve. In the case of projecting diffusion onto a straight line this does not occur since the only focal point is “hidden” at infinity. Even if the effect of infinite effective diffusion can be avoided when projecting diffusion onto a straight line, it might be unavoidable in the case of projecting diffusion along a geodesic on surfaces like the sphere. The mathematical explanation for this is that the sphere is a compact surface, but the plane is not.

4. Finite transversal diffusion rate cases

In this section we will deduce two new formulas for the effective diffusion coefficient that improve the estimation obtained in the previous section. To do this we will apply a technique described by Kalinay & Percus in [6]. The idea consists in approximating the original channel by a simpler one, and estimating the effective diffusion coefficient by finding an explicit stable solution of the diffusion
equation with the appropriate boundary conditions on the simpler channel. We will incorporate this idea into our work by using complex analytic functions as follows.

Recall that real and imaginary parts of a complex analytic function are stable solutions of the diffusion equation, i.e. they are harmonic functions. Let $\Omega$ be the channel region and suppose that we can find an explicit formula for a complex analytic function on $\mathcal{P}: \Omega \to \mathbb{C}$ whose real part has zero flux along the upper and lower walls of $\Omega$. By the Cauchy-Riemann equations this condition is equivalent to the imaginary part of $\mathcal{P}$ being constant on the upper and lower walls of $\Omega$. From the results of the previous section we have that the effective density (2.2) for the real part of $\mathcal{P}$ is the real part of the complex valued function

$$\rho(u) = \int_{-1}^{1} \mathcal{P}(\varphi(u,v)) (1 - (v_0(u) + vw(u)/2) k) (w(u)/2) dv.$$  

Since the real and imaginary parts of $\mathcal{P}$ satisfy the Cauchy-Riemann equations

$$\nabla(\text{Im}(\mathcal{P})) = i\nabla(\text{Re}(\mathcal{P})),$$
we can compute the effective flux (2.4) of $\text{Re}(P)$ as follows
\[
 j(u) = -D_0 \int_{-1}^{1} \left< i\nabla(\text{Re}(P)), \frac{\partial \varphi}{\partial v}(u,v) \right> dv
 = -D_0 \int_{-1}^{1} \left< \nabla(\text{Im}(P)), \frac{\partial \varphi}{\partial v}(u,v) \right> dv
 = -D_0 \text{Im}(\mathcal{P}(\varphi(u,1)) - \mathcal{P}(\varphi(u,-1))).
\]

If we equate this flux with the one in the generalized Fick-Jacob’s equation (3.5), i.e
\[
 j(u) = -D(u)\sigma(u) \frac{\partial}{\partial u} \left( \frac{\text{Re}(\rho(u))}{\sigma(u)} \right),
\]
we obtain the following formula for the effective diffusion coefficient
\[
 D(u) = D_0 \frac{\text{Im}(D_1(u))}{\text{Re}(D_2(u))},
\]
where
\[
 D_1(u) = \mathcal{P}(\alpha_2(u)) - \mathcal{P}(\alpha_1(u))
\]
and
\[
 D_2(u) = \sigma(u) \frac{\partial}{\partial u} (\rho(u)/\sigma(u)).
\]

Equation (4.3) gives us an explicit formula for $D$ if we can compute $\mathcal{P}$ explicitly and calculate the integral (4.1). Since finding $\mathcal{P}$ or solving the integral in (4.1) explicitly cannot be easily achieved in general, we will estimate $D$ by computing $\mathcal{P}$ for a secondary channel that approximates locally the original one.

Remark. The Riemann Mapping Theorem states that if $\Omega \subset \mathbb{C}$ is open and simply connected, then there exists a bi-holomorphism $F : \Omega \rightarrow A$, where $A$ is the unit disk in $\mathbb{C}$. If we knew such a map $F$ we could define $\mathcal{P}(z) = \log(F(z))$.

4.1. Linear Case. To simplify notation we will write
\[
 \alpha'_1 = \frac{\partial \alpha_1}{\partial u}, \alpha'_2 = \frac{\partial \alpha_2}{\partial u}, v'_0 = \frac{\partial v_0}{\partial u} \text{ and } w' = \frac{\partial w}{\partial u}.
\]

For a fixed value of $u \in [u_1, u_2]$ we will approximate the channel $\Omega$ by a channel having lower and upper walls formed by the tangent lines $l_1$ and $l_2$ to the curves $\alpha_1$ and $\alpha_2$ (see Figure 4.1). If the lines $l_1$ and $l_2$ intersect at the point $p$ then the imaginary part of the function
\[
 \mathcal{P}(z) = \log(z-p) = \log(|z-p|) + i \arg(z-p)
\]
is constant along $l_1$ and $l_2$, and hence its real part is a harmonic function having zero flux on these lines.

Remark. If we more generally we chose $\mathcal{P}(z) = a \log(z-p) + b$ for $a, b \in \mathbb{R}$, our formula for $D$ turns out to be independent of $a, b$.

From the geometry of Figure 4.1 we obtain that
\[
 \text{Im}(D_1) = \arg(\alpha_2(u) - p) - \arg(\alpha_1(u) - p),
\]
\[
 = \arg(\alpha'_2(u)) - \arg(\alpha'_1(u)),
\]
i.e the quantity \( \text{Im}(\mathcal{D}_1) \) is the angle \( \theta \) between \( l_1 \) and \( l_2 \). To compute \( \mathcal{D}_2 \) we need to compute \( \rho \) explicitly. To do this we will approximate the base curve \( \alpha \) by its circle of curvature at the point of interest, which amounts to assuming that

\[
\alpha(u) = f - i \exp(iku)/k, \tag{4.8}
\]

so that

\[
N(u) = i \exp(iku).
\]

By computing the integral (4.1) we obtain

\[
\rho(u) = Q_2(u) \log(\alpha_2(u) - p) - Q_1(u) \log(\alpha_1(u) - p) - R(u),
\]

where

\[
R(u) = \frac{k}{2N^2(u)} (\alpha_2(u) - \alpha_1(u))(f - p - (\alpha_0(u) - f)),
\]

\[
Q_1(u) = \frac{k}{2N^2(u)} (\alpha_1(u) - p)(f - p - (\alpha_1(u) - f)),
\]

\[
Q_2(u) = \frac{k}{2N^2(u)} (\alpha_2(u) - p)(f - p - (\alpha_2(u) - f)).
\]

If we substitute the above formula for \( \rho \) in equation (4.5) we obtain

\[
\mathcal{D}_2(u) = R(u) + (Q_2(u) - Q_1(u)) \log \left( \frac{\alpha_2(u) - p}{\alpha_1(u) - p} \right), \tag{4.9}
\]
where
\[ R = \frac{k(\alpha_0 - f - (f - p))(\alpha_1 - f)\alpha'_1 - (\alpha_2 - f)\alpha'_2)}{2N^2(\alpha_0 - f)} \]
and
\[ Q_1 = \frac{k(f - p - (\alpha_1 - f))(\alpha_2 - f)(\alpha_1 - p)\alpha'_2}{2N^2(\alpha_2 - \alpha_1)(\alpha_0 - f)}, \]
\[ Q_2 = \frac{k(f - p - (\alpha_2 - f))(\alpha_1 - f)(\alpha_2 - p)\alpha'_1}{2N^2(\alpha_2 - \alpha_1)(\alpha_0 - f)}. \]

Having computed \( D_1 \) and \( D_2 \) explicitly we can compute \( D \) by using formula (4.3).

Observe that our formulas for \( D_1 \) and \( D_2 \) involve purely geometric quantities associated to the curves \( \alpha_1, \alpha_2 \) and \( \alpha \).

**Recovering the case of projection onto a straight line.** We can recover the formula for the effective diffusion coefficient obtained by L. Dagdug and I. Pineda [2] as a particular case of ours in the limiting case when \( k = 0 \), i.e. by projecting diffusion onto a straight line. More precisely, observe that the curve \( \alpha \) defined by (4.8) above satisfies
\[ f = \frac{i}{k} \implies \lim_{k \to 0} \alpha(u) = u, \]
so that the straight line given by the \( u \)-axis can be seen as a limiting case of the curve \( \alpha \) when \( k \to 0 \).

On the other hand, from the formulas for \( Q_1, Q_2 \) and \( R \) above, and letting \( f = i/k \), we can compute
\[ \lim_{k \to 0} R = \frac{i(\alpha'_1 - \alpha'_2)}{\alpha_1 - \alpha_2}, \]
\[ \lim_{k \to 0} (Q_2 - Q_1) = \frac{i((\alpha_2 - p)\alpha'_1 - (\alpha_1 - p)\alpha'_2)}{\alpha_1 - \alpha_2}. \]

The velocity vectors \( \alpha'_1 \) and \( \alpha'_2 \) are connected by the fact that they are obtained by sweeping the normal line of \( \alpha \) along the curve \( \alpha_1 \) and \( \alpha_2 \). This property and the fact that for \( k = 0 \) we have that \( \alpha(u) = u \) imply that
\[ \lim_{k \to 0} (Q_2 - Q_1) = 0, \]
and hence
\[(4.10) \quad D_2 = i(\alpha'_1 - \alpha'_2). \]

On the other hand, in order to express \( D_1 \) and \( D_2 \) in terms of \( w' \) and \( v'_0 \) we differentiate formulas (3.2) and (3.3) to obtain
\begin{align}
(4.11) \quad \alpha'_1 &= (1 - (v'_0 - w'/2)k)T + (v'_0 - w'/2)N, \\
(4.12) \quad \alpha'_2 &= (1 - (v'_0 + w'/2)k)T + (v'_0 + w'/2)N.
\end{align}

From these equations and formula (4.6) we obtain that
\[ \text{Im}(D_1) = \arctan \left( \frac{v'_0 + w'/2}{1 - (v'_0 + w'/2)k} \right) - \arctan \left( \frac{v'_0 - w'/2}{1 - (v'_0 - w'/2)k} \right) \]
which for \( k = 0 \) becomes
\[ \text{Im}(D_1)|_{k=0} = \arctan (v'_0 + w'/2) - \arctan (v'_0 - w'/2). \]
Similarly, from \(4.10\) and the above equations for \(\alpha_1'\) and \(\alpha_2'\) conclude that

\[ D_{2}|_{k=0} = w'. \]

Thus

\[ D|_{k=0} = D_0 \frac{\text{Im}(D_1)|_{k=0}}{\text{Re}(D_2)|_{k=0}} = D_0 \left( \frac{\arctan (v_0' + w'/2) - \arctan (v_0' - w'/2)}{w'} \right), \]

which is the formula given in \(\mathbb{P}\).

An example. To illustrate the behavior of the formula just obtained for \(D\), we study the following example. Consider the curve

\[ \alpha(u) = \frac{i}{k} (1 - \exp(iu)) \]

representing the circle of radius \(1/k\) centered at \(i/k\). Let \(\alpha_1\) and \(\alpha_2\) be the straight lines intersecting at the point \(p = -1\) and with slopes \(m_1\) and \(m_2\). We are interested in visualizing \(D\) at \(u = 0\) (see the upper left picture in Figure 4.2) where

\[ \alpha(0) = 0, N(u) = i, \alpha_1(0) = m_1 i \text{ and } \alpha_2(0) = m_2 i. \]

Let \(l_k\) be the straight line joining the focal point \(f = i/k\) and 1. If we place the vectors \(\alpha_1'(0)\) and \(\alpha_2'(0)\) at the points \(\alpha_1(0)\) and \(\alpha_2(0)\) respectively, they have their end points at the intersections of \(l_k\) with \(l_1\) and \(l_2\). This geometric condition can be written algebraically as follows

\[ \alpha_1'(0) = \frac{(1 + im_1)(1 - km_1)}{1 + km_1}, \]

\[ \alpha_2'(0) = \frac{(1 + im_2)(1 - km_2)}{1 + km_2}. \]

Substituting the above formulas in our formula for \(D\), we obtain \(D\) as a function of \(m_1, m_2\) and \(k\). In figure 4.2 we show the geometric setting of the above description for the values \(k = 0, 0.2, 1.6\) and 2.5. Figure 4.3 we show the resulting effective diffusion coefficient \(D\) as a function of \(m_1\) and \(m_2\) for the same values of \(k\). Observe that as \(k\) gets bigger, the focal point \(f\) approaches the line \(l_2\) and \(D\) tends to become singular.

4.2. Quadratic case. In this case, we approximate the curves \(\alpha_1, \alpha_2\) and \(\alpha\) by their corresponding circles of curvature \(C_1, C_2\) and \(C\) (see Figure 4.4).

We will estimate the effective diffusion coefficient by studying the effective flux of a stationary solution of the two dimensional diffusion equation that has no flux across \(C_1\) and \(C_2\). As in the previous sub-section, we will let \(\alpha : [-\pi/k, \pi/k] \to \mathbb{C}\) be the arc-length parametrization of the circle \(C\) of radius \(1/k\) and centre \(f\) given by

\[ \alpha(u) = f - i \exp(iu)/k, \]

and the upper and lower walls of our channel \(\Omega\) will be circles \(C_1\) and \(C_2\) with radii \(1/k_1, 1/k_2\) and centers \(f_1, f_2\), respectively. The channel \(\Omega\) can be parametrized (at least locally) by a map \(\varphi : [-\pi/k, \pi/k] \times [-1, 1] \to \mathbb{C}\) of the form

\[ \varphi(u, v) = \alpha(u) + (v_0(u) + v w(u)/2) N(u), \]

where the functions \(v_0\) and \(w\) are implicitly defined by the equations

\[ |\alpha_1(u) - f_1| = 1/k_1 \text{ and } |\alpha_2 - f_2| = 1/k_2, \]
and \( N \), the unit normal field to the circle \( C \), is given by

\[ N(u) = \exp(iku). \]

The middle curve is given by

\[ \alpha_0(u) = \varphi(u, 0) = \alpha(u) + v_0(u)N(u), \]

and the circles \( C_1 \) and \( C_2 \) have parametrizations

\[
\begin{align*}
\alpha_1(u) &= \varphi(u, -1) = \alpha(u) + (v_0(u) - w(u)/2)N(u), \\
\alpha_2(u) &= \varphi(u, 1) = \alpha(u) + (v_0(u) + w(u)/2)N(u).
\end{align*}
\]

In Appendix 2 we show how to find points \( q_1, q_2 \) in \( \mathbb{C} \) such that the imaginary part of the function (see formulas (6.4) and (6.5))

\[
\mathcal{P}(z) = \begin{cases} 
I \log \left( \frac{(z + q_1)}{(z - q_2)} \right) & \text{for } f_1 \neq f_2, \\
i \log (z - g) & \text{for } f_1 = f_2 = g.
\end{cases}
\]
is constant on $C_1$ and $C_2$ (see Figure 4.2), and where the coefficient $I$ is defined by

$$I = \begin{cases} i & \text{if } C_1 \cap C_2 = \emptyset, \\ 1 & \text{if } C_1 \cap C_2 \neq \emptyset. \end{cases}$$

The real part of $\mathcal{P}$ is then a stationary solution (i.e. time-independent) of the two-dimensional diffusion equation that has no flux across $C_1$ or $C_2$. We will first consider the case $f_1 \neq f_2$. Using this $\mathcal{P}$ in the integral (4.1) we obtain

$$\rho = Q_2 \log(\alpha_2 - q_1) - Q_1 \log(\alpha_1 - q_1) + Q_4 \log(\alpha_2 - q_2) - Q_3 \log(\alpha_1 - q_2) - R,$$
Figure 4.4. Approximation by circular channel

where

\[ Q_1 = kI((\alpha_1 - q_1 - 2f)(\alpha_1 - q_1) - \alpha_1 - q_1) \]
\[ Q_2 = kI((\alpha_2 - q_1 - 2f)(\alpha_2 - q_1) - \alpha_2 - q_1) \]
\[ Q_3 = kI((\alpha_1 - q_2 - 2f)(\alpha_1 - q_2) - \alpha_1 - q_2) \]
\[ Q_4 = kI((\alpha_2 - q_2 - 2f)(\alpha_2 - q_2) - \alpha_2 - q_2) \]
\[ R = \frac{kI(q_2 - q_1)(\alpha_2 - \alpha_1)}{2n^2} \]

By using the above formula for \( \rho \), we obtain

\[ D_2 = Q(q_2) \log \left( \frac{\alpha_2 - q_2}{\alpha_1 - q_2} \right) - Q(q_1) \log \left( \frac{\alpha_2 - q_1}{\alpha_1 - q_1} \right) \]

where

\[ Q(z) = \frac{kI(\alpha_1 + z - 2f)(\alpha_1 - z)(\alpha_2 - f)\alpha'_2}{2n^2(\alpha_2 - \alpha_1)(\alpha_0 - f)} - \frac{(\alpha_1 - f)(\alpha_2 + z - 2f)(\alpha_2 - z)\alpha'_1}{2n^2(\alpha_2 - \alpha_1)(\alpha_0 - f)} \]
\[ R(z) = \frac{kI(q_2 - q_1)((\alpha_2 - f)\alpha'_2 - (\alpha_1 - f)\alpha'_1)}{2n^2(\alpha_0 - f)} \]
For the case $f_1 = f_2 = g$ we need to use the function
\[ \mathcal{P}(z) = i \log(z - g) \]
from which we obtain
\[ \rho = R - (Q_2 \log(\alpha_2 - g) - Q_1 \log(\alpha_1 - g)) \]
where
\begin{align*}
Q_1 &= \frac{ik(\alpha_1 + g - 2f)(\alpha_1 - g)}{2N^2} , \\
Q_2 &= \frac{ik(\alpha_2 + g - 2f)(\alpha_2 - g)}{2N^2} , \\
R &= \frac{ik(\alpha_0 + g - 2f)(\alpha_2 - \alpha_1)}{2N^2} .
\end{align*}
Using this formula for $\rho$ we obtain
\[ D_2 = Q \log \left( \frac{\alpha_2 - g}{\alpha_1 - g} \right) - R, \]
where
\begin{align*}
Q &= \frac{ik((\alpha_1 + g - 2f)(\alpha_1 - g)(\alpha_2 - f)\alpha_2')}{2N^2(\alpha_2 - \alpha_1)(\alpha_0 - f)} - \frac{(\alpha_2 + g - 2f)(\alpha_2 - g)(\alpha_1 - f)\alpha_1')}{2N^2(\alpha_2 - \alpha_1)(\alpha_0 - f)} , \\
R &= \frac{ik(\alpha_0 + g - 2f)((\alpha_2 - f)\alpha_2' - (\alpha_1 - f)\alpha_1')}{2N^2(\alpha_0 - f)} .
\end{align*}
Recovering the case of infinite transversal diffusion rate for symmetric channels of constant width. In this case the circles of curvature of $\alpha_1, \alpha_2$ and $\alpha$ have the same center, namely the center of curvature $f$ of $\alpha$. Hence, we can assume that
\begin{align*}
\alpha(u) &= f - i \exp(iku)/k , \\
\alpha_1(u) &= f - i \exp(iku)/k_1 , \\
\alpha_2(u) &= f - i \exp(iku)/k_2 .
\end{align*}
If we substitute these formulas in equations (4.13) and (4.14) and let $g = f$ we get
\[ D_1 = i \log(k_1/k_2) \quad \text{and} \quad D_2 = \frac{k^2}{2} \left( \frac{1}{k_1^2} - \frac{1}{k_2^2} \right) . \]
By using formula (5.1) we obtain
\[ k_1 = \frac{k}{1 - kw/2} \quad \text{and} \quad k_2 = \frac{k}{1 + kw/2} \]
and hence
\[ D_1 = i \log \left( \frac{1 + kw/2}{1 - kw/2} \right) \quad \text{and} \quad D_2 = kw . \]
We conclude that
\[ D = \frac{D_0}{kw} \log \left( \frac{1 + kw/2}{1 - kw/2} \right) , \]
which is formula (3.7) for the infinite transversal diffusion case. In other words, the infinite transversal diffusion rate formula is actually a second order approximation.
for symmetric constant width channels. This results is reasonable since in this case the upper and lower curve follows the base curve “as closely as possible”.

5. Appendix - A brief review of the differential geometry of plane curves.

In this appendix we review some basic concepts of the differential geometry of plane curves. The material is standard and can be found in books such as [8, 3]. Consider a smooth planar curve parametrized by a function $\alpha : [s_1, s_2] \to \mathbb{R}^2$ where $\alpha(s) = (x(s), y(s))$. The curve is said to have arc-length parametrization if for all $s$ in the interval $[s_1, s_2]$ we have that

$$\left| \frac{d\alpha}{ds} \right| = 1 \quad \text{where} \quad \left| \frac{d\alpha}{ds} \right| = \sqrt{\left( \frac{dx}{ds} \right)^2 + \left( \frac{dy}{ds} \right)^2}.$$

If the above condition holds, then the length of the curve segment $\alpha([s_1, s])$ is given by

$$\text{length}(\alpha([s_1, s])) = \int_{s_1}^{s} \left| \frac{d\alpha}{ds}(a) \right| da = s.$$

In this case we have that $T = \left( \frac{dx}{ds}, \frac{dy}{ds} \right)$ and $N = \left( -\frac{dy}{ds}, \frac{dx}{ds} \right)$ are the unit tangent and unit normal fields to $\alpha$. Since $T$ has unit length its derivative must be a scalar multiple of $N$, i.e

$$\frac{dT}{ds} = kN.$$

The resulting function $k : [s_1, s_2] \to \mathbb{R}$ is known as the curvature function of $\alpha$. Similarly

$$\frac{dN}{ds} = -kT.$$

For $k(u) \neq 0$ the point

$$f(u) = \alpha(u) + \frac{1}{k(u)} N(u)$$

is known as the focal point of $\alpha$ at $u$, and the scalar $r(u) = 1/k(u)$ is known as the radius of curvature. The circle with centre $f(u)$ and radius $r(u)$ is an approximation of second order to the curve $\alpha$ at the point $\alpha(u)$. The set of focal points is known as the focal curve. The families of curves $\alpha_v(u) = \alpha(u) + vN(u)$ and $\beta_u(v) = \alpha(u) + vN(u)$ form an orthogonal system of curves that becomes degenerate at the focal curve of $\alpha$ (see Figure 5.1). The curves $\alpha_v$ share the same focal curve, and the curvature function $k_v$ of $\alpha_v$ can be computed as

$$k_v = \frac{k}{1 + kv}.$$

If the curve $\alpha$ is not parametrized by the arc-length parameter $s$ but by an arbitrary parameter $t$, we can calculate the curvature function of $\alpha$ by the following formula

$$k = \left( \frac{\partial x}{\partial t} \frac{\partial^2 y}{\partial t^2} - \frac{\partial y}{\partial t} \frac{\partial^2 x}{\partial t^2} \right) / \left( \left( \frac{\partial x}{\partial t} \right)^2 + \left( \frac{\partial y}{\partial t} \right)^2 \right)^{3/2}.$$
6. Appendix - A complex analytic function whose real part has zero flux across a pair of arbitrary circles

The purpose of this appendix is to derive an explicit formula for a complex analytic function \( P : \mathbb{C} \rightarrow \mathbb{C} \) whose real part has zero flux across two arbitrary planar circles \( C_1 \) and \( C_2 \). By the Cauchy-Riemann equations this last condition is equivalent to the imaginary part of \( P \) having \( C_1 \) and \( C_2 \) as level sets. We will denote the centers of \( C_1 \) and \( C_2 \) by \( f_1 \) and \( f_2 \), and their radii by \( r_1 \) and \( r_2 \). The desired function will have the form

\[
P(z) = \mathcal{I} \log \left( \frac{z - q_2}{z - q_1} \right) = \mathcal{I} \left( \log \left| \frac{z - q_2}{z - q_1} \right| + i \arg \left( \frac{z - q_2}{z - q_1} \right) \right),
\]

where \( \mathcal{I} \) is the imaginary unit.
Figure 6.1. Steiner Net.

for adequate values of $q_1$ and $q_2$ in $\mathbb{C}$, and where

$$I = \begin{cases} i & \text{if } C_1 \cap C_2 = \emptyset, \\ 1 & \text{if } C_1 \cap C_2 \neq \emptyset. \end{cases}$$

We will first study the case when both $q_1$ and $q_2$ are real numbers with $q_1 = -q_2$ and initially assume that $C_1 \cap C_2 = \emptyset$. We will then explain how to obtain the general case from this one.

For $q \geq 0$, we will write $q_1 = q$, $q_2 = -q$ so that

$$P(z) = i \log \left( \frac{z + q}{z - q} \right).$$

The solutions of the equations

\begin{align*}
(6.1) & \quad \text{Im}(P(z)) = \log(\alpha), \\
(6.2) & \quad \text{Re}(P(z)) = \theta,
\end{align*}

define a net of circles known as the Steiner net (see Figure 6.1). The radius $r$ and
center $c$ of a circle defined by equation 6.1 are given by

$$r = \frac{2q\alpha}{|\alpha^2 - 1|} \quad \text{and} \quad c = q \left( \frac{\alpha^2 + 1}{\alpha^2 - 1} \right).$$

We can solve these equations for $\alpha$ and $f$ to obtain

$$\alpha = \sqrt{q^2 + r^2} \pm \frac{q}{r},$$

where the choice of signs must be the same in both formulas, and the sign determines if the corresponding circle of radius $r$ lies on the positive or negative side of the real axis. Hence, for any $q$ the circles radii $r_1$ and $r_2$ correspond to the values

$$\alpha_1 = \frac{\sqrt{q^2 + r_1^2} \pm q}{r_1} \quad \text{and} \quad \alpha_2 = \frac{\sqrt{q^2 + r_2^2} \pm q}{r_2}.$$

We can fix the distance $d = |c_2 - c_1|$ between the centers of the circles by letting

$$(6.3) \quad q = \frac{1}{2d} \sqrt{(d^2 - (r_1 + r_2)^2)(d^2 - (r_2 - r_1)^2)},$$

Having chosen this $q$ we can recover the centers of the circles by the formulas

$$c_1 = \pm \sqrt{q^2 + r_1^2} \quad \text{and} \quad c_2 = \pm \sqrt{q^2 + r_2^2}.$$

We will choose $c_1$ to be positive. If $c_2$ is negative the circles are outside each other, and if $c_2$ is positive then one circle is inside of the other. It turns out that for $q$ given by (6.3) a small correction to our formula for $P$ will even work for the case when $q$ is complex. This last condition corresponds to the case when $C_1$ and $C_2$ intersect (see Figure 6.2). In order to introduce the needed correction, we will need the functions

$$\mathcal{I} = \begin{cases} 
    i & \text{if } q \text{ is real,} \\
    1 & \text{if } q \text{ is complex.}
\end{cases}$$

and

$$\mathcal{J} = \begin{cases} 
    1 & \text{if } (\mathcal{I} = 1 \text{ and } d < c_1) \text{ or } (\mathcal{I} = i \text{ and } d < r_1 + r_2) \\
    -1 & \text{otherwise}
\end{cases}$$

Our final formula, which deals with the case of general $q_1$ and $q_2$ can be obtained by using the transformation

$$T(z) = \frac{(c_2 - c_1)z + c_1f_2 - c_2f_1}{f_2 - f_1}$$

that satisfies $T(f_1) = c_1, T(f_2) = c_2$. For $d = |f_2 - f_1|$ and $q$ given by equation (6.3) the function with the desired properties is

$$P(z) = \mathcal{I} \log \left( \frac{z - q_1}{z - q_2} \right),$$

where

$$c_1 = \sqrt{q^2 + r_1^2}, c_2 = \mathcal{J} \sqrt{q^2 + r_2^2}.$$
For $f_1 = f_2$ (i.e. $d = 0$) the function $P$ is not well defined. We correct this by letting

$$P(z) = \begin{cases} \mathcal{I}\log((z - q_2)/(z - q_1)) & \text{for } f_1 \neq f_2, \\ i\log(z - g) & \text{for } f_1 = f_2 = g. \end{cases}$$

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