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Diffusion in a curved tube

Naohisa Ogawa *

Hokkaido Institute of Technology, Teine, Sapporo 006-8585, Japan

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ABSTRACT

The diffusion of particles in confining walls forming a tube is discussed. Such a transport phenomenon is observed in biological cells and porous media. We consider the case in which the tube is winding with curvature and torsion, and the thickness of the tube is sufficiently small compared with its curvature radius. We discuss how geometrical quantities appear in a quasi-one-dimensional diffusion equation.

1. Introduction

To control the transportation of micro- and nanoparticles artificially, it is very important to understand the diffusion properties under the confining walls. These phenomena are encountered in biological cells [1] and zeolite [2], and in catalytic reactions in porous media [3]. For this purpose, the diffusion properties in confined geometries are discussed by several authors. The diffusion in a membrane with a certain thickness is discussed by Gov [4], Gambin et al. [5], and Ogawa [6]. The diffusion in general curved manifold is discussed by Castro-Villarreal [7]. The diffusion in a tube with a varying cross section along the axis (channel model) is discussed by Jacobs [8], Yanagida [9], Zwanzig [10], Reguera and Rubi [11], and Kalinary and Percus [12], and as a review, see Burada et al. [13]. Surprisingly, this channel model is related to the reaction rate theory due to the Smoluchowski equation [13,14].

In this Letter, we discuss the case in which a tube has a fixed cross section but is winding with geometrical properties, namely, curvature and torsion. Then, we show that the diffusion in such a tube with a Neumann boundary condition can be expressed by a quasi-one-dimensional diffusion equation with an effective diffusion coefficient that depends on curvature. This is carried out by integrating a three-dimensional diffusion equation in the cross section of the tube. The coefficient depends on the curvature of the central line of the tube. The physical interpretation of its curvature dependence is given by analogy to Ohm's law.

By using the obtained equation, we show the mean square displacement (MSD) of torus and helix tubes where the curvature is constant. When the curvature depends on position, we show the short time expansion for MSD.

In Section 2, we introduce the curvilinear coordinates and related metrics in a winding tube. This is carried out by using Frenet–Seret (FS) equations explained in Appendix A. In Section 3, we define the quasi-one-dimensional diffusion field. In Section 4, the diffusion equation is obtained by using a local equilibrium condition. This condition is an assumption that the diffusion in the same cross section is completed in a short time, which is much smaller than our observed time scale; thus, we may assume that the density is flat on the same cross section. In Section 5, we discuss the diffusion equation beyond the local equilibrium condition. In Section 6, we calculate MSD from the quasi-one-dimensional diffusion equation and show first two terms in the short time expansion by using curvature and its derivatives. In Section 7, the conclusion is given.

2. Metric in tube

We consider the quasi-one-dimensional diffusion equation as the limitation process from a three-dimensional usual diffusion equation in a thin tube with a circular cross section. We set the curved tube with the radius ϵ in the three-dimensional Euclidean space R_3. The curvilinear coordinates that specify the points in the tube and their bases we use hereafter are as follows (see Fig. 1).

$\vec{X}$ is the Cartesian coordinate in R_3. s $(=q^1)$ is the length parameter along the center line of the tube and $\vec{e}_1$ is its tangential vector. $\vec{x}(s)$ is the Cartesian coordinate that specifies the points on the center line. q^i is the coordinate in the transversal direction $\vec{e}_i$, the small Latin indices $i, j, k, \ldots$ run from 2 to 3 and the Greek indices $\mu, \nu, \ldots$ run from 1 to 3. We sometimes use the

* Tel.: +81 116882291.
E-mail address: ogawanao@hit.ac.jp.

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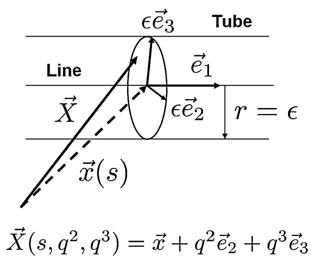

Fig. 1. Local orthogonal coordinates $\{s, q^2, q^3\}$ in tube.

notations $s = q^1$, $v = q^2 = r\cos\theta$, and $w = q^3 = r\sin\theta$ to obtain simpler expressions, and we define the area element of the cross section $d\sigma = dv\,dw = r\,dr\,d\theta$. $\vec{e}_1, \vec{e}_2$, and $\vec{e}_3$ are the unit basis vectors introduced by the Frenet–Seret equations [15,16] explained in Appendix A. Then, we identify any points in the tube using

$$\vec{X}(s, q^2, q^3) = \vec{x}(s) + q^i \vec{e}_i(s), \tag{1}$$

where $0 \leqslant |\vec{q}| \leqslant \epsilon$ with $|\vec{q}| = \sqrt{(q^2)^2 + (q^3)^2}$.

From this relation, we obtain the curvilinear coordinate system in the tube ($\subset R_3$) using the coordinate $q^\mu = (q^1, q^2, q^3)$ and metric $G_{\mu\nu}$:

$$G_{\mu\nu} = \frac{\partial \vec{X}}{\partial q^\mu} \cdot \frac{\partial \vec{X}}{\partial q^\nu}. \tag{2}$$

$G_{\mu\nu}$ is calculated by using the Frenet–Seret equations (Appendix A):

$$G_{\mu\nu} = \begin{pmatrix} 1 - 2\kappa v + (\kappa^2 + \tau^2)v^2 + \tau^2 w^2 & -\tau w & \tau v \\ -\tau w & 1 & 0 \\ \tau v & 0 & 1 \end{pmatrix}, \tag{3}$$

where κ is the curvature and τ is the torsion defined in Appendix A. We have nonzero off-diagonal elements due to the existence of torsion. The determinant of the metric tensor does not depend on torsion:

$$G \equiv \det(G_{\mu\nu}) = (1 - \kappa v)^2. \tag{4}$$

The inverse metric is given as

$$G^{\mu\nu} = \frac{1}{(1 - \kappa v)^2} \times \begin{pmatrix} 1 & \tau w & -\tau v \\ \tau w & (1 - \kappa v)^2 + (\tau w)^2 & -\tau^2 v w \\ -\tau v & -\tau^2 v w & (1 - \kappa v)^2 + (\tau v)^2 \end{pmatrix}. \tag{5}$$

3. Diffusion field in tube

Let us define a three-dimensional diffusion field by $\phi^{(3)}$ and a three-dimensional Laplace–Beltrami operator with metric tensor (3) by $\hat{\Delta}$. Then, we obtain the diffusion equation with a normalization condition:

$$\frac{\partial \phi^{(3)}}{\partial t} = D \hat{\Delta} \phi^{(3)}, \tag{6}$$

$$N = \int \phi^{(3)}(q^1, q^2, q^3) \sqrt{G}\, d^3 q, \tag{7}$$

where D is the diffusion constant, $G \equiv \det(G_{\mu\nu})$, and N is the number of particles. Our aim is to construct the effective one-dimensional diffusion equation from the 3D equation above in a small radius limit:

$$\frac{\partial \phi^{(1)}}{\partial t} = D \hat{\Delta}^{(eff)} \phi^{(1)}, \tag{8}$$

$$N = \int \phi^{(1)}(s)\, ds, \tag{9}$$

where $\phi^{(1)}$ is the one-dimensional diffusion field and $\hat{\Delta}^{(eff)}$ is the unknown effective 1D diffusion operator that might not be equal to the simple 1D Laplace–Beltrami operator $\partial^2/\partial s^2$.

From two normalization conditions, namely, (7) and (9), we obtain

$$\begin{aligned} N &= \int \phi^{(3)}(q^1, q^2, q^3) \sqrt{G}\, d^3 q \\ &= \int \left[\int dq^2 dq^3 \left(\phi^{(3)} \sqrt{G} \right) \right] ds \\ &= \int \phi^{(1)}(s)\, ds. \end{aligned}$$

The particle number between s and $s + ds$ should be equal in the two fields. Thus, we obtain

$$\phi^{(1)}(s) = \int \phi^{(3)} \sqrt{G}\, dq^2\, dq^3. \tag{10}$$

We multiply $\sqrt{G}$ by Eq. (6) and integrate it by q^2 and q^3 to obtain

$$\frac{\partial \phi^{(1)}}{\partial t} = D \int (\sqrt{G} \hat{\Delta}) \phi^{(3)}\, dq^2\, dq^3. \tag{11}$$

From the form of the Laplace–Beltrami operator

$$\Delta = G^{-1/2} \frac{\partial}{\partial q^\mu} G^{1/2} G^{\mu\nu} \frac{\partial}{\partial q^\nu},$$

our diffusion equation has the form

$$\begin{aligned} \frac{\partial \phi^{(1)}}{\partial t} &= D \int \frac{\partial}{\partial q^\mu} G^{1/2} G^{\mu\nu} \frac{\partial}{\partial q^\nu} \phi^{(3)}\, d\sigma \\ &= D \frac{\partial}{\partial s} \int \frac{1}{\sqrt{G}} \left(\frac{\partial}{\partial s} - \tau \frac{\partial}{\partial \theta} \right) \phi^{(3)}\, d\sigma, \end{aligned} \tag{12}$$

where the Neumann boundary condition is used at the second equality. The torsion appears only when the axial symmetry of $\phi^{(3)}$ is broken as is expected from the definition.

4. Local equilibrium condition

The fluctuation mode in the cross section decreases with time like $\exp(-Dt/\epsilon^2)$, and only the zero mode (uniform in the same cross section) survives at $t \gg \epsilon^2/D$, i.e. the equilibrium is realized in the transverse direction in a short time. Then we suppose the "local equilibrium condition" as

$$\frac{\partial \phi^{(3)}}{\partial q^i} = 0, \quad i = 2, 3. \tag{13}$$

This condition works out for straight tube or flat sheet with width ϵ evidently. But it is not so clear in the case with large curvature. In this sense it is still a hypothesis at this stage to use (13), however, we come back to this problem in the next section and we have a consistent result.

In the following we restrict our observation in the time scale t satisfying $t \gg \epsilon^2/D$ and we assume the local equilibrium condition (13). Note that this condition includes the Neumann condition at the boundary of the tube.

From Eqs. (10) and (13), we also obtain

$$\phi^{(3)} = \frac{\phi^{(1)}}{\sigma}, \qquad \sigma \equiv \int \sqrt{G}\, d\sigma = \pi \epsilon^2. \tag{14}$$