Geometric Flow in Diffusion and Quantum Mechanics on Surface with Thickness

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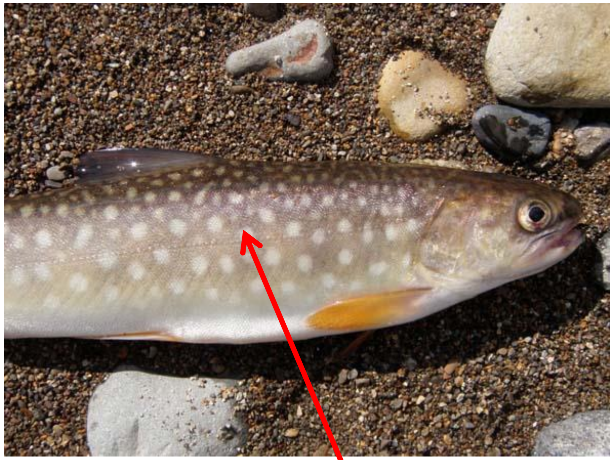
Talk at June 2018, Varna Bulgaria

Motivation

How do we obtain the skin pattern of fish?

Char Fish



white spot pattern

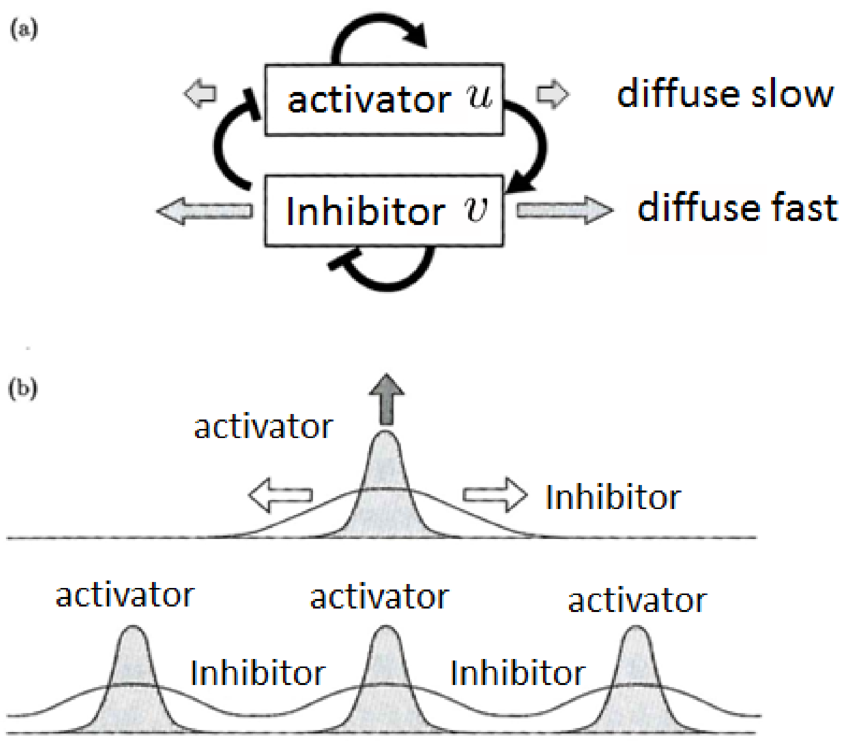
(Side Face)

Labyrinth pattern

(Dosal)

Patterns are constructed by Reaction Diffusion Equation

Two or more kinds of chemical matters that diffuse with chemical reaction give rise to various patterns!



Activator

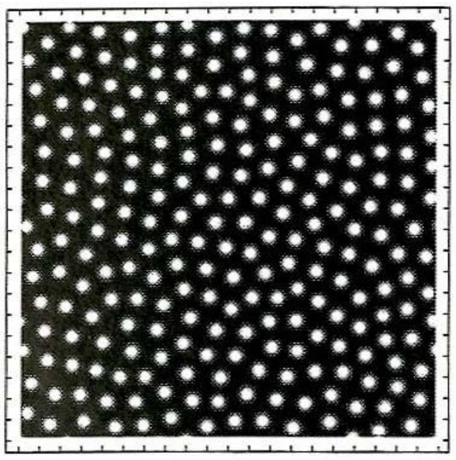
$$\frac{\partial u}{\partial t} = au - bv + D_u \Delta u,$$

Inhibitor

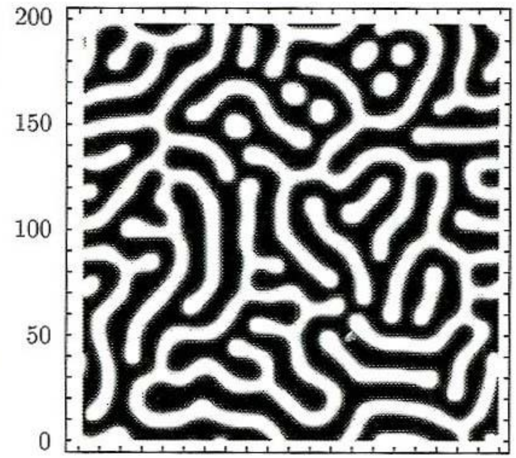
$$\frac{\partial v}{\partial t} = cu - dv + D_v \Delta v.$$

$$a > 0,\ b > 0,\ c > 0,\ d > 0,\quad D_v >> D_u.$$

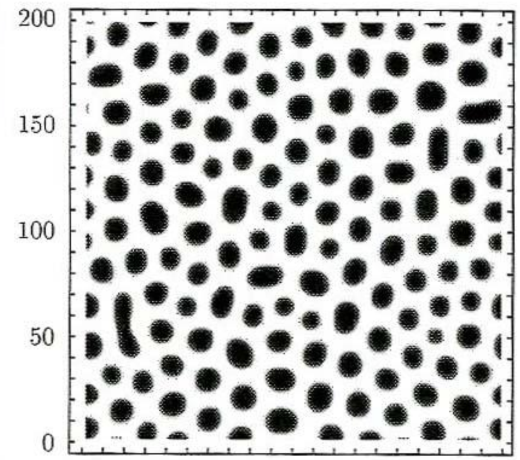
Patterns given by reaction diffusion



White Spots



Labyrinth



Black Spots

“Mathematical Biology” J.D. Murray

The Effects of curvature seems to be appeared on the skin of Char fish

Dorsal part:

Large mean curvature

⇒ Labyrinth pattern

Side face part:

Small mean curvature

⇒ Spot pattern

** Surface of fish can be approximated by elliptic cylinder -> NO Gaussian curvature.

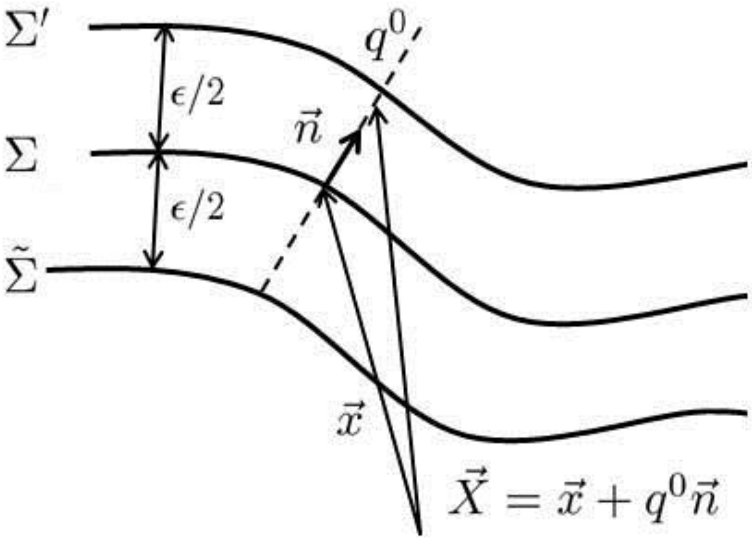
How can we realize such an idea that the pattern change induced by curvature?

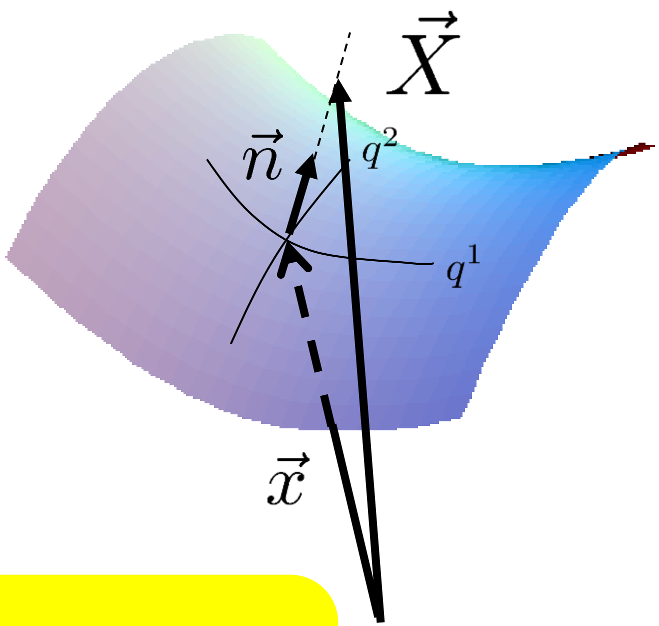
We need to consider the matter diffusion on surface that depends on curvature

Starting from the surface diffusion, there's no contribution of mean curvature.

We start with surface with thickness ϵ, and consider the 3D diffusion eq., and transcribe to the effective 2D diffusion eq..

Particle diffusion in thin space sandwiched by two surfaces

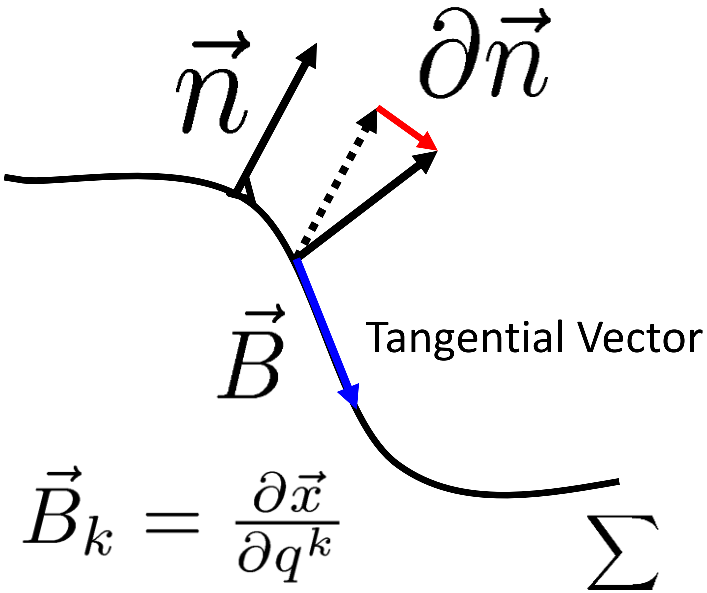




$$\vec{X}(q^0, q^1, q^2) = \vec{x}(q^1, q^2) + q^0\vec{n}$$

$$-\epsilon/2 \leq q^0 \leq \epsilon/2$$

Geometrical Tools



$$\vec{B}_k = \frac{\partial \vec{x}}{\partial q^k}$$

1st Fundamental Tensor (Metric)

$$g_{ij} = \vec{B}_i \cdot \vec{B}_j$$

2nd Fundamental Tensor

$$\kappa_{ij} = \frac{\partial \vec{n}}{\partial q^i} \cdot \vec{B}_j$$

Mean Curvature: $$\kappa = \sum_{i,j=1}^{2} g^{ij} \kappa_{ij}$$

Gaussian Curvature: $$G \equiv R/2 = det(\sum_{k=1}^{2} g^{ik} \kappa_{kj}) = det(\kappa^i_j)$$

Effective 2-Dimensional Diffusion Equation

$$-\frac{\partial \phi}{\partial t} = \sum_{i=1}^{2} \nabla_i (J^i + J_A^i)$$

Covariant Derivative

$$J^i = -D \sum_{j=1}^{2} g^{ij} \frac{\partial \phi}{\partial q^j}$$

Fick's Law

$$J_A^i = -\frac{D\epsilon^2}{12} \sum_{j=1}^{2} \{ (3\kappa^{im}\kappa_m^j - 2\kappa\kappa^{ij}) \frac{\partial \phi}{\partial q^j} - \frac{1}{2} g^{ij} \frac{\partial R}{\partial q^j} \phi \}$$

$$+\mathcal{O}(\epsilon^4)$$

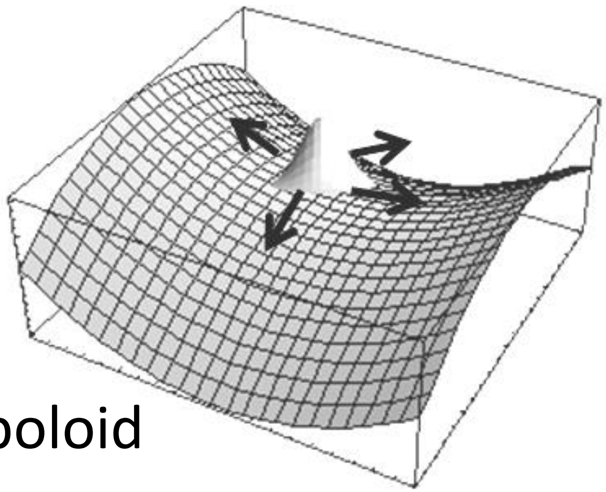
(curvature dep. coefficient)

Positive: Diffusion
Negative:Concentration

Drift due to
Curvature gradient

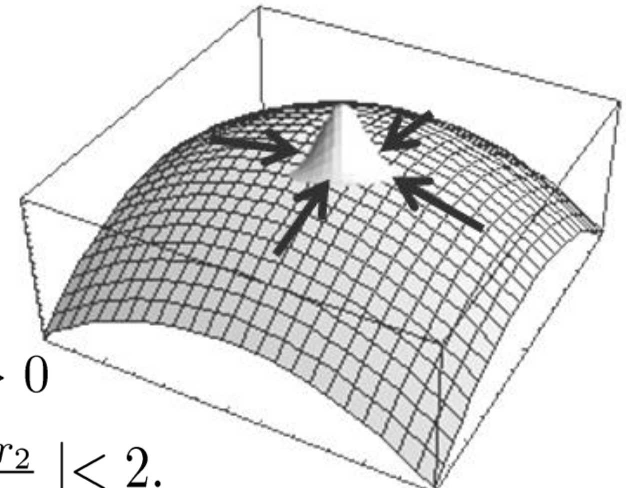
N. Ogawa : Phys.Rev. E81, 2010

The Anomalous Flow
(Diffusion and Concentration)



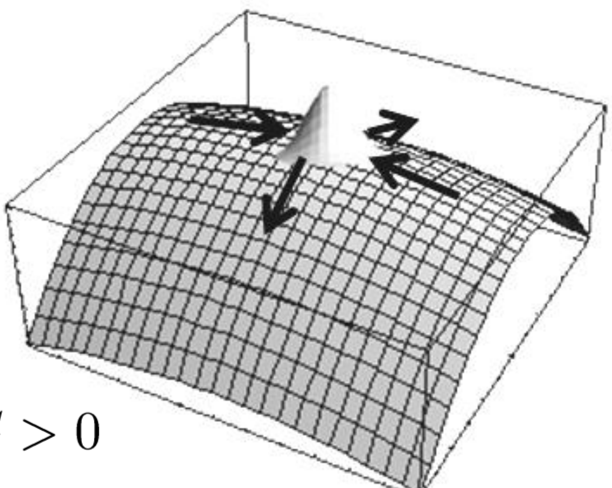
$G < 0$

hyperboloid



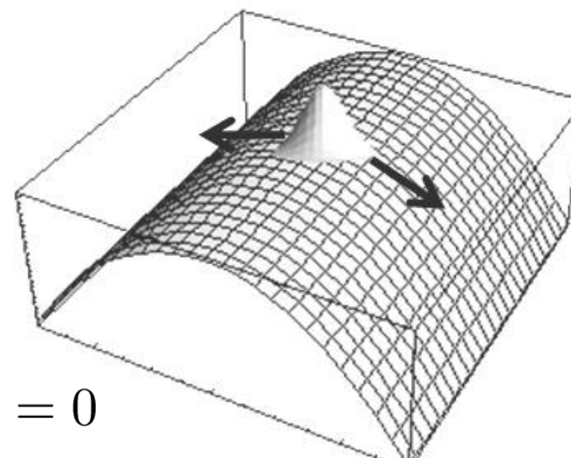
$G > 0$

$1/2 < \left| \frac{r_2}{r_1} \right| < 2.$



$G > 0$

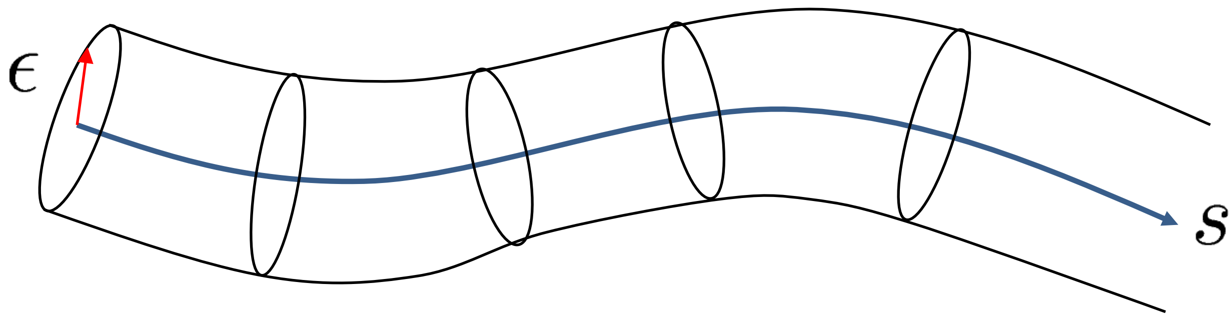
$\left| \frac{r_2}{r_1} \right| < 1/2, \text{ or } \left| \frac{r_2}{r_1} \right| > 2.$



$G = 0$

G: Gaussian Curvature

Line with Thickness : Tube (One dimensional case)



We have an effective 1D diffusion equation in exact form!

$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial s} D_{eff}(s) \frac{\partial}{\partial s} \phi$$

$$D_{eff} = D\left(1 + \left(\frac{\kappa\epsilon}{2}\right)^2 + \mathcal{O}(\epsilon^4)\right) = 2D\frac{1 - \sqrt{1 - (\kappa\epsilon)^2}}{(\kappa\epsilon)^2}$$

$$\kappa = \frac{1}{R}, \quad R \text{ is curvature radious of central line.}$$

N. Ogawa, Phys. Lett. 2013

Mean square Displacement in Curved Tube

At t=0, particles are set at s=0, $\phi(t=0,s)=\delta(s).$
then the mean square displacement is given by

$$< s^2 >= a_1 t + a_2 t^2 + \cdots$$

$$a_1 = \frac{\partial < s^2 >}{\partial t}\bigg|_{t=0} = 2 < D_{eff}(s) >_{t=0} + 2 < s\ D'_{eff}(s) >_{t=0} = 2D_{eff}(0).$$

$$a_2 = \frac{1}{2}\frac{\partial^2 < s^2 >}{\partial t^2}\bigg|_{t=0} = 3D''_{eff}(0)D_{eff}(0) + D'_{eff}(0)^2.$$

Where, $D_{eff}(s) = 2D\frac{1-\sqrt{1-(\kappa(s)\epsilon)^2}}{(\kappa(s)\epsilon)^2}$

Applications

We are still working for fish skin pattern by simulation, but having other applications:

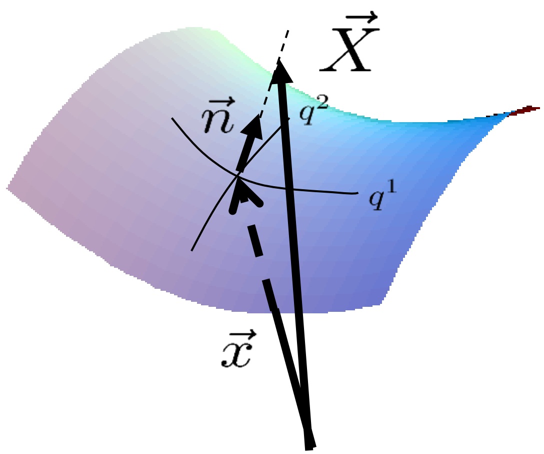
(1) Growth and transport inside the epidermis (melanocytic lesions) medical science group

(2) The Diffusion of molecules in Lipid bilayer

Quantum Mechanics on Surface with Thickness

Remember our coordinate setting:

Curvilinear Coordinate $q^\mu = \{q^0, q^1, q^2\}$



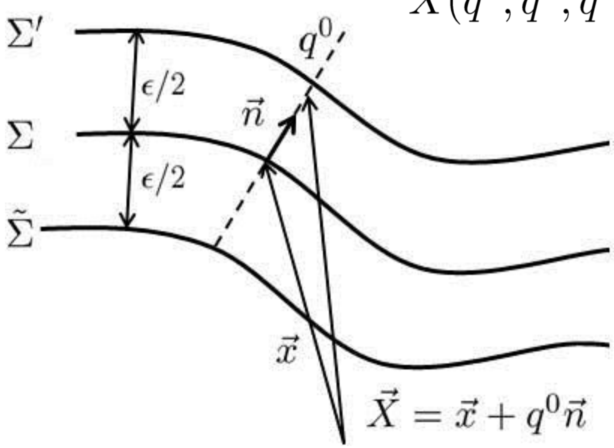
1st, 2nd fundamental tensors on Σ

$$g_{ij} = \frac{\partial \vec{x}}{\partial q^i} \cdot \frac{\partial \vec{x}}{\partial q^j} \quad \kappa_{ij} = \frac{\partial \vec{n}}{\partial q^i} \cdot \frac{\partial \vec{x}}{\partial q^j}$$

Metric around Σ: $G_{\mu\nu} = \frac{\partial \vec{X}}{\partial q^\mu} \cdot \frac{\partial \vec{X}}{\partial q^\nu}$

$$\vec{X}(q^0, q^1, q^2) = \vec{x}(q^1, q^2) + q^0 \vec{n}$$

$$G_{\mu\nu} = \begin{pmatrix} 1 & 0 \\ 0 & G_{ij} \end{pmatrix}.$$



$$-\epsilon/2 \le q^0 \le \epsilon/2$$

$$G_{ij} = g_{ij} + q^0\left(\frac{\partial \vec{x}}{\partial q^i} \cdot \frac{\partial \vec{n}}{\partial q^j} + \frac{\partial \vec{x}}{\partial q^j} \cdot \frac{\partial \vec{n}}{\partial q^i}\right) + (q^0)^2 \frac{\partial \vec{n}}{\partial q^i} \cdot \frac{\partial \vec{n}}{\partial q^j} \quad (i, j = 1, 2)$$

$$G_{ij} = g_{ij} + 2q^0 \kappa_{ij} + (q^0)^2 \kappa_{im} \kappa_j^m$$

Schrödinger Equation in Curved Surface with thin Layer

Schrödinger equation with curvi-linear coordinate:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta^{(3)}\psi + V(q^1, q^2)\psi$$

Laplace Beltrami operator

$$\Delta^{(3)} \equiv G^{-1/2}\partial_\mu G^{1/2} G^{\mu\nu}\partial_\nu$$

Normalization Condition

combined as $|\tilde{\psi}|^2$

$$1 = \int |\psi|^2\sqrt{G}d^3q = \int [\int_{-\epsilon/2}^{+\epsilon/2} |\psi|^2\sqrt{\frac{G}{g}}\, dq^0]\sqrt{g}d^2q$$

Now we rewrite the equation with new variable $\tilde{\psi}$ with normalization condition:

$$\int [\int_{-\epsilon/2}^{+\epsilon/2} |\tilde{\psi}|^2 dq^0]\sqrt{g}d^2q = 1, \qquad \tilde{\psi} \equiv (G/g)^{1/4}\psi$$

normalization condition relation

New Schrödinger equation

$$i\hbar\frac{\partial\tilde{\psi}}{\partial t} = -\frac{\hbar^2}{2m}\tilde{\Delta}^{(3)}\tilde{\psi} + V\tilde{\psi}$$

$$\tilde{\Delta}^{(3)} \equiv (G/g)^{1/4}\Delta^{(3)}(G/g)^{-1/4}$$

$$1 = \int |\tilde{\psi}|^2\sqrt{g}d^3q = \int [\int_{-\epsilon/2}^{+\epsilon/2} |\tilde{\psi}|^2 \ dq^0]\sqrt{g}d^2q$$

Note: We suppose that *V* does NOT depend on q^0

Decomposition of new Laplacian

$$\tilde{\Delta}^{(3)} = \Delta^{(2)} + \frac{\partial^2}{\partial (q^0)^2} + \underline{V_0} + q^0 V_1 + (q^0)^2 V_2 + q^0 \hat{A}_1 + (q^0)^2 \hat{A}_2 + \mathcal{O}((q^0)^3)$$

Effect of Embedding remains even for $\epsilon \to 0$
R.C.T.da Costa, Phys.Rev. 23 (1981),1982

$$V_0 = \frac{1}{4}(\kappa^2 - 2R)$$

$$V_1 = \kappa(R - \frac{\kappa^2}{2}) - \frac{1}{2}\Delta^{(2)}\kappa$$

$$V_2 = \frac{3}{4}\kappa^4 - \frac{7}{4}\kappa^2 R + \frac{1}{2}R^2 + \frac{1}{2}\kappa\Delta^{(2)}\kappa + \frac{1}{4}g^{ij}(\partial_i\kappa)(\partial_j\kappa) + \nabla_i(\kappa^{ij}\partial_j\kappa) - \frac{1}{4}\Delta^{(2)}R$$

$$\hat{A}_1 = -2\nabla_i \kappa^{ij}\partial_j$$

$$\hat{A}_2 = 3\nabla_i \kappa^{ik}\kappa_k^j \partial_j$$

Diff. Op

$$\partial_j \equiv \frac{\partial}{\partial q^j}, \qquad (j = 1, 2)$$

∇_j (Covariant Derivative)

Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_I,$$

$$\begin{aligned}
\hat{H}_0 &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(q^0)^2} - \frac{\hbar^2}{2m}[\Delta^{(2)} + V_0] + V, \\
\hat{H}_I &= -\frac{\hbar^2}{2m}[q^0(V_1 + \hat{A}_1) + (q^0)^2(V_2 + \hat{A}_2) + (\mathrm{H.O.})].
\end{aligned}$$

States in normal motion

In Low Energy case, N=1 is enhanced, so we have

$$\chi_1 = \sqrt{\frac{2}{\epsilon}} \cos(\pi q^0/\epsilon) =< q^0|\chi_1 >, \quad E_1 = \frac{\hbar^2 \pi^2}{2m\epsilon^2}$$

We neglect the transition to other higher states since it occurs at higher order in perturbation.

$$\frac{< \chi_n|\hat{H}_I|\chi_1 >}{E_n - E_1}\Big|_{n\neq 1} \sim \frac{\mathcal{O}(\epsilon)}{1/\epsilon^2} = \mathcal{O}(\epsilon^3)$$

We consider the theory up to $\mathcal{O}(\epsilon^2)$

Eigen states for $\hat{H}_0$

$$i\hbar\frac{\partial}{\partial t}\psi = \hat{H}_0\psi, \qquad \psi_{n,\alpha} = \chi_n(q^0)\phi_\alpha(q^1, q^2)e^{-i(E_n+\epsilon_\alpha)t}.$$

Separation of variable method

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(q^0)^2}\chi_n(q^0) = E_n\ \chi_n(q^0), \quad E_n = \frac{\hbar^2\pi^2n^2}{2m\epsilon^2}, \ n = 1, 2, 3\cdots$$

with solution
$$\chi_n = \begin{cases} \sqrt{2}\cos(n\pi q^0/\epsilon) & n = \text{odd}, \\ \sqrt{2}\sin(n\pi q^0/\epsilon) & n = \text{even}. \end{cases}$$

Schrödinger equation on Σ : $(-\frac{\hbar^2}{2m}[\Delta^{(2)} + V_0] + V)\phi_\alpha = \epsilon_\alpha\phi_\alpha.$

Normalization: $\int \chi_n^*(q^0)\chi_m(q^0)dq^0 = \delta_{nm}, \quad \int \phi_\alpha^*(q)\phi_\beta(q)\sqrt{g}dq^1dq^2 = \delta_{\alpha,\beta}$

Effective Hamiltonian up to $\mathcal{O}(\epsilon^2)$

Then we have effective Hamiltonian and state for other variables $q^1, \quad q^2$ by omitting the transition to upper state.

$$\begin{aligned}
\hat{H}_{eff} &\equiv < \chi_1|\hat{H}|\chi_1 > \\
&= -\frac{\hbar^2}{2m}[\Delta^{(2)} + V_0] + V + E_1 \\
&\quad -\frac{\hbar^2}{2m}[< \chi_1|q^0|\chi_1 > (V_1 + \hat{A}_1) + < \chi_1|(q^0)^2|\chi_1 > (V_2 + \hat{A}_2)].
\end{aligned}$$

$$< \chi_1|q^0|\chi_1 > = \int |\chi_1(q^0)|^2 q^0 dq^0 = 0,$$

$$< \chi_1|(q^0)^2|\chi_1 > = \int |\chi_1(q^0)|^2 (q^0)^2 dq^0 = \frac{\epsilon^2}{2\pi^2}(\frac{\pi^2}{6} - 1)$$

Effective Schrödinger Equation

$$i\hbar\frac{\partial\phi}{\partial t} = -\frac{\hbar^2}{2m}[\Delta^{(2)} + V_0 + < (q^0)^2 > (V_2 + \hat{A}_2)]\phi + V\phi$$

$$= -\frac{\hbar^2}{2m}[\Delta^{(2)} + < (q^0)^2 > \hat{A}_2)]\phi + V_{all}\phi$$

$$\hat{A}_2 = 3\nabla_i\kappa^{ik}\kappa^j_k\partial_j, \quad < (q^0)^2 >= \frac{\epsilon^2}{2\pi^2}(\frac{\pi^2}{6} - 1)$$

Then we obtain conservation law of probability

$$-\frac{\partial|\phi|^2}{\partial t} = \nabla_i\tilde{J}^i \qquad \tilde{J}^i = J^i + J^i_A$$

Anomalous Current

$$-\frac{\partial|\phi|^2}{\partial t} = \nabla_i \tilde{J}^i \qquad \tilde{J}^i = J^i + J^i_A$$

$$J^i = \frac{\hbar}{2mi}\, g^{ij}(\phi^*\partial_j\phi - \phi\partial_j\phi^*),$$

$$J^i_A = \frac{\hbar}{2mi}\frac{3\epsilon^2}{2\pi^2}\left(\frac{\pi^2}{6} - 1\right)\, \kappa^i_k\kappa^{kj}(\phi^*\partial_j\phi - \phi\partial_j\phi^*)$$

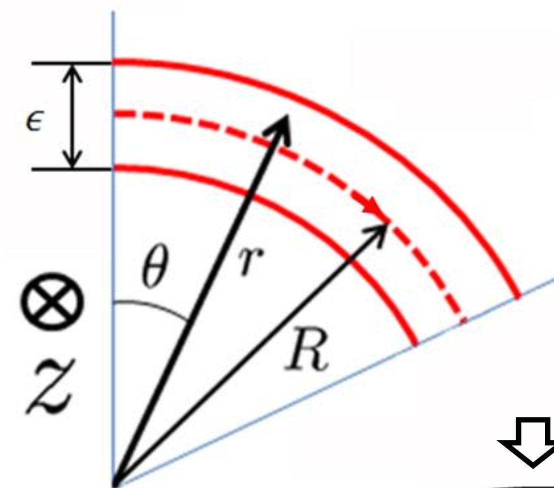
Anomalous Geometric Current

We can prove that $\kappa^i_k\kappa^{kj}$ can be diagonal , and eigenvalues are not negative.

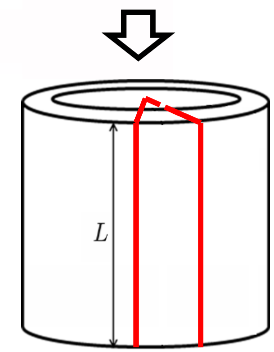
One Example of Anomalous Current

Consider the part of cylinder with thickness ϵ such as,

$$R - \epsilon/2 < r < R + \epsilon/2, \quad 0 < z < L.$$



Top View



In this 3D region, the conservation law is written in cylindrical coordinate (r, θ, z)

$$ds^2 = dr^2 + r^2 d\theta^2 + dz^2, \quad G_{\mu\nu} = \mathrm{diag}(1, r^2, 1)$$

$$\nabla_\mu \tilde{J}^\mu = -\frac{\partial \tilde{\rho}}{\partial t}, \quad \text{conservation law}$$

$$\tilde{J}^\mu = \frac{\hbar}{2mi} G^{\mu\nu} (\psi^* \nabla_\nu \psi - \psi \nabla_\nu \psi^*),$$

$$\tilde{\rho} = |\psi|^2.$$

$$\tilde{J}^r = \frac{\hbar}{2mi}(\psi^* \partial_r \psi - \psi \partial_r \psi^*),$$

$$\tilde{J}^\theta = \frac{\hbar}{2mr^2 i}(\psi^* \partial_\theta \psi - \psi \partial_\theta \psi^*),$$

$$\tilde{J}^z = \frac{\hbar}{2mi}(\psi^* \partial_z \psi - \psi \partial_z \psi^*).$$

$$\partial_\theta \tilde{J}^\theta + \partial_r \tilde{J}^r + \partial_z \tilde{J}^z + \frac{1}{r}\tilde{J}^r = -\partial_t \tilde{\rho}.$$

Integrate B.H.S. by $\int_{R-\epsilon/2}^{R+\epsilon/2} dr r$ we obtain,

$$\partial_\theta J^\theta + \partial_z J^z = -\partial_t \rho, \qquad \int \rho \, d\theta dz = 1,$$

$$J^\theta \equiv \int_{R-\epsilon/2}^{R+\epsilon/2} r\tilde{J}^\theta \, dr, \quad J^z \equiv \int_{R-\epsilon/2}^{R+\epsilon/2} r\tilde{J}^z \, dr, \quad \rho \equiv \int_{R-\epsilon/2}^{R+\epsilon/2} r\tilde{\rho} \, dr,$$

$$\boxed{J^\theta = \frac{\hbar}{2mi} \int_{R-\epsilon/2}^{R+\epsilon/2} \frac{dr}{r} (\psi^* \partial_\theta \psi - \psi \partial_\theta \psi^*)}$$

By using

$$\psi(r, \theta, z) = (g/G)^{1/4} \underbrace{\varphi(\theta, z)\chi(r)}_{\tilde{\psi}} = \sqrt{\frac{R}{r}} \varphi(\theta, z)\chi(r)$$

$$\int_{R-\epsilon/2}^{R+\epsilon/2} |\chi|^2 dr = 1, \quad \int |\varphi|^2 R d\theta dz = 1$$

We obtain

$$J^\theta = \frac{\hbar R}{2mi} \underline{\int_{R-\epsilon/2}^{R+\epsilon/2} \frac{dr}{r^2} |\chi(r)|^2} (\varphi^* \partial_\theta \varphi - \varphi \partial_\theta \varphi^*) = \frac{\hbar R}{2mi} < \frac{1}{r^2} > (\varphi^* \partial_\theta \varphi - \varphi \partial_\theta \varphi^*)$$

$$J^\theta = \frac{\hbar R}{mi\epsilon}\int_{-\epsilon/2}^{+\epsilon/2}\frac{dq^0}{(R+q^0)^2}\cos^2(\pi q^0/\epsilon),$$
$$\times\left(\varphi^*\partial_\theta\varphi - \varphi\partial_\theta\varphi^*\right),$$

$$\frac{1}{(R+q^0)^2} = \frac{1}{R^2}\frac{1}{(1+(q^0/R))^2} = \frac{1}{R^2}(1 - 2(q^0/R) + 3(q^0/R)^2 + \cdots)$$

contributes to normal current

This term contributes to anomalous current

On the other hand,

$$J^z = \frac{\hbar}{2mi}\left(\int_{R-\epsilon/2}^{R+\epsilon/2} dr\ |\chi(r)|^2\right)(\varphi^*\partial_z\varphi - \varphi\partial_z\varphi^*)$$
$$= \frac{\hbar}{2mi}(\varphi^*\partial_z\varphi - \varphi\partial_z\varphi^*).$$

In straight direction, we have no anomalous current

Anomalous current appears from the average treatment in thickness direction in higher order in ϵ

Conclusion

Classical

$$-\frac{\partial \phi}{\partial t} = \nabla_i (J^i + J^i_A)$$

$$J^i = -D g^{ij} \frac{\partial \phi}{\partial x^j}$$

$$J^i_A = -\frac{D\epsilon^2}{12} \{ (3\kappa^{im} \kappa^j_m - 2\kappa\kappa^{ij}) \frac{\partial \phi}{\partial q^j} - \frac{1}{2} g^{ij} \frac{\partial R}{\partial q^j} \phi \}$$

Quantum

$$-\frac{\partial |\phi|^2}{\partial t} = \nabla_i (J^i + J^i_A)$$

$$J^i = \frac{\hbar}{2mi} \; g^{ij} (\phi^* \partial_j \phi - \phi \partial_j \phi^*),$$

$$J^i_A = \frac{\hbar}{2mi} \frac{3\epsilon^2}{2\pi^2} (\frac{\pi^2}{6} - 1) \; \kappa^{im} \kappa^j_m (\phi^* \partial_j \phi - \phi \partial_j \phi^*)$$

References

(1) B. Alberts, A. Johnson , M. Raff M, K. Roberts, P. Walter , Molecular Biology of the Cell, Garland, N.Y. 2007;

(2) J.D. Murray, Mathematical Biology, Springer; 3rd Corrected ed. 2002. Corr. 3rd printing 2008

(3) P. Burada, P. Hanggi, F. Marhesoni, G. Schmid, P. Talkener, Diffusion in Confined Geometries, Chem. Phys. Chem. 10 (2009)

(4) P. Castro-Villarreal, Brownian Motion meets a Riemannian Curvature, J. Stat. Mech. (2010)

(5) R. da Costa, Phys.Rev. A23 (1981) (On quantum potential)

(6) N. Ogawa, K. Fujii, A.Kobushkin, N.M. Chepilko, P.T.P 83(1990); P.T.P 85(1991):P.T.P 87(1992)

(7)N.Ogawa, Phys.Rev.E81 (2010) (diffusion on surface with thickness)

(8)N.Ogawa, Phys. Lett. A377,(2013) (diffusion in curved Tube)

Thank you for your attention

Appendix on diffusion

We suppose the local equilibrium in normal direction

$$\frac{\partial \phi}{\partial q^0} = 0$$

Reason:

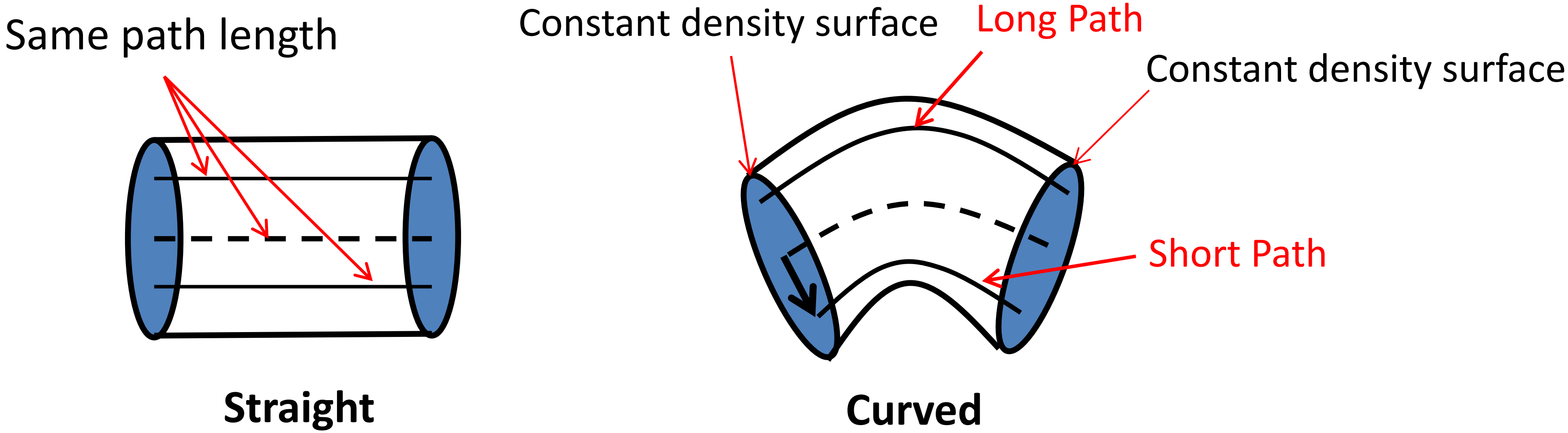
As the relaxation time $\tau = \epsilon^2/D$ is much shorter than the our observing time scale, we can suppose the equilibrium holds into normal direction. Furthermore, this condition is consistent with Neumann condition in diffusion process.

$$\frac{\partial \phi}{\partial q^0}|_{\pm\epsilon/2} = 0$$

Even for such a condition, we still have curvature effect.

Why do we have a curvature effect?

At curved points, diffusion effect is large!



This is similar to the following electric circuit !

$$R_{tot} = \frac{R}{3}$$

$$R_{tot} \sim \frac{R}{3} - \frac{2r^2}{9R}$$