Diffusion in almost-Riemannian geometry 3/3

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We have seen the definition of 2-ARS as the generalized Riemannian structure obtained locally by declaring that a pair of vector fields satisfying the Hormander condition is an orthonormal frame

 $\rightarrow \mathrm{if}$ the orthonormal frame is global we say that it is \mathbf{free}

We have seen

- properties of the singular set
- type of points (Riemannian Grushin and Tangency) and normal forms
- Geodesics: they are smooth and can cross the singular set, but
 - spheres of finite diameter can have infinite (Riemannian) volume and infinite (Riemannian) perimeter
 - a conjugate locus could be present even if the curvature is always negative where it is defined

A Gauss Bonnet Theorem

Theorem (Gauss-Bonnet)

Let M be a 2D, compact, orientable Riemannian manifold. Then $\int_M K dA = 2\pi \ \chi(M) = 2\pi (2-2\mathbf{g})$

can we extend such a result in the AR context?

Of course this cannot be done directly. For instance for 2-step structures we have that $K \to -\infty$ on the singular set.

Definition

A 2-ARS is orientable if **U** is orientable as vector bundle.

Roughly this is equivalent to ask that we can take all matrices of changes of orthonormal frames in SO(2).

$$Y_1(q) = \cos(\theta)X_1(q) + \sin(\theta)X_2(q),$$

$$Y_2(q) = -\sin(\theta)X_1(q) + \cos(\theta)X_2(q).$$

 \rightarrow This concept is unrelated from the orientability of M.

 \rightarrow There exists non orientable structures on orientable manifolds and viceversa.

Definition

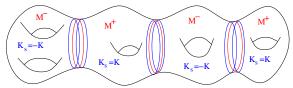
- A 2-ARS is fully orientable if
 - it is orientable
 - and M is orientable.

Definition

Consider a **fully-orientable**, **2-step** 2-ARS. Let $\omega \in \Lambda^2(M)$ be a never vanishing two-form, defining an orientation on M. Define

$$M^{\pm} = \{ p \in \Omega_i \setminus \mathcal{Z} | i \in I, \pm \omega(X_i, Y_i)(p) > 0 \}$$
(1)

We call signed curvature the function (defined on $M \setminus \mathcal{Z}$) $\frac{K_s(p)}{K_s(p)} = \begin{cases} K(p), & \text{if } p \in M^+, \\ -K(p), & \text{if } p \in M^-, \end{cases}$ (2)



For every $\varepsilon > 0$, let $M_{\varepsilon} = \{p \in M | d(p, \mathcal{Z}) > \varepsilon\}$ We say that K_s is integrable on M if

$$\lim_{\varepsilon \to 0} \int_{M_{\varepsilon}} K_s \, dA \tag{3}$$

exists and is finite. In this case we denote such limit by $\int \mathcal{K}_s dA$.

Theorem

Consider a fully-orientable, 2-step 2-ARS. Then

$$\mathcal{K}_s dA = 2\pi (\chi(M^+) - \chi(M^-)), \tag{4}$$

where χ denotes the Euler characteristic.

Lemma

If M is orientable and the 2-step 2-ARS is free (\Rightarrow fully orientable) then $(\chi(M^+) - \chi(M^-)) = 0.$

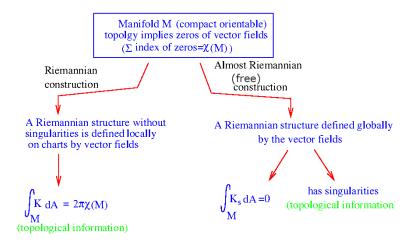
Corollary

Let M be a compact oriented two-dimensional manifold and consider a free 2-step 2-ARS on it. Then

$$\int \mathcal{K}_s dA = 0 \tag{5}$$

This is a deep fact: If the metric is defined globally by a couple of vector fields, then $\int \mathcal{K}_s dA = 0$. This is what happens in Riemannian geometry: on the torus!

 \rightarrow we "force the manifold to be parallelizable by accepting singularities"



(only) on the torus the two constructions coincide

If the structure is not free one can prove that

$$\chi(M^+) - \chi(M^-) = e(\mathbf{U})$$

Where $e(\mathbf{U})$ is the Euler number of U. and then

Theorem

Consider a fully-orientable, 2-step 2-ARS. Then

$$\int \mathcal{K}_s dA = 2\pi e(\mathbf{U}) \tag{6}$$

Extensions in presence of tangency points are possible, but less natural.

Diffusion and Schroedinger evolution on 2-ARS

How to define the heat and the Schroedinger equation in a 2-ARS?

$$\partial_t \phi = \frac{1}{2} \Delta \phi, \qquad i \partial_t \phi = -\frac{\hbar^2}{2} \Delta \phi$$

What is the right operator Δ ?

 $\Delta = X_1^2 + X_2^2$ is not a good choice because

■ it is not invariant by change of orthonormal frame

• it is not global if the structure cannot be defined with one frame only To have an invariant operator the simplest thing is to look for an operator of the form

$$\Delta = \operatorname{div}_{\omega} \circ \operatorname{grad}$$

(the definition of grad extends with no difficulties to ARSs)

The problem is the choice of ω . We have $\infty + 1$ choices

- either we choose from outside a regular volume $\omega \Rightarrow$ we get a well defined hypoelliptic operator but then the diffusion will depend on ω
- or we take the Riemannian area dA. In this case we obtain the **Laplace-Beltrami** operator which diverges on \mathcal{Z} .

in 2-ARS an intrinsic volume which is not diverging is not known (in a sense it does not exist)

Let us start to study the (diverging) Laplace Beltrami operator

 $\Delta = \operatorname{div}_{dA} \circ \operatorname{grad} = X_1^2(\phi) + X_2^2(\phi) + \operatorname{div}(X_1)X_1(\phi) + \operatorname{div}(X_2)X_2(\phi)$ The first order term are diverging

For the Grushin metric $X_1 = \partial_x$, $X_2 = x \partial_y$, $dA = \frac{1}{|x|}$ and we obtain

$$\Delta \phi := \operatorname{div}_{dA}(\operatorname{grad}(\phi)) = \left(\partial_x^2 + x^2 \partial_y^2 - \frac{1}{x} \partial_x\right) \phi,$$

If we take $\omega = dx \, dy$ we obtain

 $\tilde{\Delta}\phi := \operatorname{div}_{\omega}(\operatorname{grad}(\phi)) = \left(\partial_x^2 + x^2 \partial_y^2\right)\phi,$

Is there a propagation of the heat through the singular set? (same question for the Schroedinger equation)

This question is essentially equivalent to

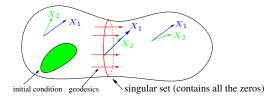
Q: Let M be a 2D manifold endowed with a 2-ARS. Let Ω be a connected component of $M \setminus \mathcal{Z}$. Let Δ be the corresponding Laplace-Beltrami defined on $C_0^{\infty}(\Omega)$. Is Δ essentially self-adjoint on $L^2(\Omega, dA)$?

 \rightarrow If Δ is essentially self-adjoint on $L^2(\Omega, dA)$ then the Cauchy problems for the heat and Schoredinger equations are well defined in $L^2(\Omega, dA)$ without the need of boundary conditions \Rightarrow no propagation.

 $\rightarrow \mathrm{If}$ it is not essentially self-adjoint then one needs boundary conditions. For instance

- Dirichlet-like conditions (killing condition)
- Neumann-like (reflecting condition)
- other conditions permitting to connect the two sides (bridging extensions see [B. Prandi 2016])

A a priori one expects a negative answer to this question (i.e. Δ is not essentially self adjoint) since a positive answer would imply that neither the heat flow, neither a quantum particle can pass through \mathcal{Z} , while classical geodesics cross it with no singularities.



Theorem (U.B, Camille Laurent, 2013)

Let M be a 2D compact orientable manifold endowed with a 2-ARS. Assume that

(H) for every
$$q \in M$$
, $\blacktriangle(q) + [\blacktriangle, \blacktriangle](q) = T_q M$.

Let Ω be a connected component of $M \setminus \mathcal{Z}$. Then Δ with domain $C_0^{\infty}(\Omega)$ is essentially self-adjoint on $L^2(\Omega, dA)$.

Remark (H) is an open condition implying that $\rightarrow Z$ is a finite union of non-intersecting circles \rightarrow only Riemannian and Grushin points are present \rightarrow the compactness hypothesis is not necessary (but simplify the statement)

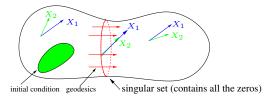
Corollary

Consider the unique solution ϕ of the Schroedinger equation,

$$i\partial_t \phi = -\frac{\hbar^2}{2} \Delta \phi \tag{7}$$

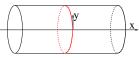
$$\phi(0) = \phi_0 \in L^2(M, dA) \tag{8}$$

with ϕ_0 supported in a connected component Ω of $M \setminus \mathcal{Z}$. Then, $\phi(t)$ is supported in Ω for any $t \geq 0$. The same holds for the solution of the heat or for the solution of the wave equation.



Idea of the proof of the self-adjointness: the Grushin cylinder

• The Grushin Cylinder is the Grushin plane in which we compactifies the *y* variable



• By setting $f = \sqrt{|x|g}$ $\partial_x^2 + x^2 \partial_y^2 - \frac{1}{x} \partial_x$ on $L^2(\frac{1}{|x|} dx dy)$ \downarrow (9) $\partial_x^2 + x^2 \partial_y^2 - \frac{3}{4} \frac{1}{x^2}$ on $L^2(dx dy)$ • By making Fourier transform in y, we are reduced to study the selfadjointness of:

$$\partial_x^2 - \frac{3}{4} \frac{1}{x^2} - k^2 x^2$$
 on $]0, \infty[$
i.e. of $-\partial_x^2 + \frac{3}{4} \frac{1}{x^2} + k^2 x^2$ on $]0, \infty[$

Proposition (Reed-Simon)

The operator $-\partial_x^2 + \frac{c}{|x|^2}$ defined on $L^2(]0, +\infty[)$ with domain $C_0^\infty(]0, +\infty[)$ is essentially self-adjoint if and only $c \geq \frac{3}{4}$.

(uses the limit-point limit circle theory Weyl's Theorem)

 \rightarrow The rest of the proof for an almost Riemannian structure consists in generalizing this result for a normal form around a connected component of the singular set and to treat it as a perturbation of the Grushin case.

Remarks

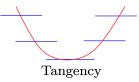
- the explosion of the area naturally acts as a barrier, which prevents the particles from crossing the degeneracy zone.
- One cannot relate the heat kernel $p_t(q_1, q_2)$ to the distance as in the Riemannian case

 $-4t \log p_t(q_1, q_2) \rightarrow d(q_1, q_2)^2$ (Varadhan '67) is not true on ARSs

■ No semiclassical theory for the Schroedinger equation

 \rightarrow such a phenomenon is today called Quantum Confinement (and there are today many further results on rank-varying Sub-Riemannian structures, see Rizzi, Prandi, Seri, Franceschi)

 \rightarrow The theorem is not proved in presence of tangency points (hard open question)

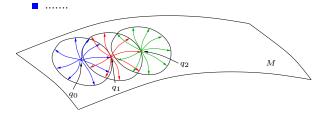


heat blocking by the Grushin singularity: a Random walk interpretation

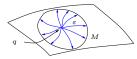
In Riemannian geometry the Laplacian can be constructed as the generator of a limit random walk.

We consider a particle that

- at time zero is in q_0 ;
- at time δt jumps on a point q_1 of the sphere of radius ε centered in q_0 , uniformly on the sphere, by following a geodesic;
- at time $2\delta t$ jumps on a point q_2 of the sphere of radius ε centered in q_1 uniformly on the sphere, by following a geodesic;



If ϕ is the density of probability of finding the particle in q we have that:



how much ϕ is increasing at a point q in time δt is proportional to the difference between the average of ϕ in a sphere of radius ε centered in q and the value of $\phi(q, t)$.

$$\phi(q,t+\delta t) - \phi(q,t) = \int_{S^{n-1}} \left(\phi\big(\exp_q(\varepsilon,\theta),t\big) - \phi(q,t) \big) d\theta.$$

Dividing by δt we obtain

$$\frac{\phi(q,t+\delta t)-\phi(q,t)}{\delta t}=\frac{1}{\delta t}\int_{S^{n-1}}\Big(\phi\big(\exp_q(\varepsilon,\theta),t\big)-\phi(q,t)\Big)d\theta.$$

Taking the parabolic scaling (\leftrightarrow infinite velocity) $\delta t = \varepsilon^2$, and for $\delta t \to 0$,

$$\partial_t \phi = L\phi, \quad \text{where } L\phi(q,t) = \lim_{\varepsilon \to 0} \underbrace{\frac{1}{\varepsilon^2} \int_{S^{n-1}} \left(\phi\left(\exp_q(\varepsilon,\theta),t\right) - \phi(q,t) \right) d\theta}_{S^{n-1}}.$$
 (10)

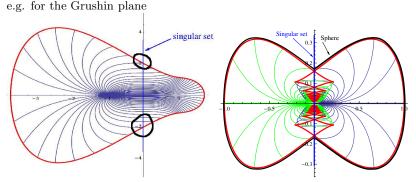
generator of the random walk

Up to constants we have

$$L = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^2} \int_{S^{n-1}} \Big(\phi \big(\exp_q(\varepsilon, \theta), t \big) - \phi(q, t) \Big) d\theta = \Delta$$

there is a way of passing from convergence of the operator to convergence of the process.

in 2D almost-Riemannian geometry the **front and the sphere are not** admissible curves when they intersect the singular set. Hence their length is infinite and the heat is trapped in the singularity!



 \rightarrow We do not have a so intuitive interpretation for the Schroedinger equation

 \rightarrow For the Grushin plane we proved that we are stochastically incomplete i.e. that

$$\int_{M} \phi(t,q) dA(q) \text{ is decreasing}$$

(the singular set is eating the heat)

 \rightarrow the quantum sphere is an example of compact manifolds (\Rightarrow geodesically complete) that is stochastically incomplete.

(in Riemannian geometry on compact manifold we are always geodesically and stochastically complete)

Schroedinger evolution

Some new results

In quantum mechanics semiclassical analysis says roughly:

• if ψ is wave packet solution of the Schroedinger equation, then for $\hbar \to 0$, its maximum satisfies the classical equation of the motion.

However the theory is delicate and on Riemannian manifolds even how to construct the quantum operator starting from the classical Hamiltonian is not obvious (the quantization procedure is not unique).

 \rightarrow there are many possible quantizations (i.e., ways of writing the Schroedinger equation starting from the classical Hamiltonian) that can be divided in two categories:

- intrinsic quantizations (usually called "geometric quantizations")
- extrinsic quantizations (using the embedding in \mathbf{R}^n)

the intrinsic approach: Geometric quantization

Literature on geometric quantization, path integrals etc. suggests that in a **Riemannian manifold** in dimension 2

where

- K(q) is the Gaussian curvature. In dimension ≥ 2 one should use the scalar curvature R (notice that R = 2K in dimension two).
- $c \ge 0$ is a constant that depends on the quantization procedure. Most used values are $c = 0, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}$. See [Andersson-Driver1999]
 - formal expansion methods: $c = \frac{1}{3}, c = \frac{1}{2}, c = \frac{2}{3};$
 - geometric quantization: $c \in [0, 2/3]$. Weyl quantization c = 0;
 - path integral: there is an ambiguity reflecting in the ambiguity of *c*.

for $\hbar \to 0$ for a Riemannian manifolds the curvature term becomes irrelevant, but for 2-ARS this is not the case since it is diverging.

For the Grushin cylinder (after the unitary transformation $L^2(\frac{1}{|x|}dx dy) \rightarrow L^2(dx dy)$)

$$\begin{split} i\hbar\partial_t\psi &= -\frac{\hbar^2}{2m}(\Delta - cK)\psi \\ &= -\frac{\hbar^2}{2m}\Big((\partial_x^2 + x^2\partial_y^2 - \frac{3}{4}\frac{1}{x^2}) - c(-\frac{2}{x^2})\Big)\psi \\ &= \frac{\hbar^2}{2m}\Big(-(\partial_x^2 + x^2\partial_y^2) + \frac{3}{4}\frac{-2c}{x^2}\Big)\psi \end{split}$$

 \rightarrow Clearly for c = 3/8 the divergence term disappear and we are not essentially self-adjoint in $\mathbf{R}^+ \times \mathbf{R}$.

 \rightarrow Actually all c > 0 destroy the self-adjointness because $\frac{3}{4} - 2c > \frac{3}{4}$ (remember the Reed-Simon theorem).

Theorem

Let M be a 2D compact orientable manifold endowed with a 2-ARS. Assume that

(H) for every
$$q \in M$$
, $\blacktriangle(q) + [\blacktriangle, \blacktriangle](q) = T_q M$.

Let Ω be a connected component of $M \setminus \mathcal{Z}$. Then $\Delta - cK(q)$ with domain $C_0^{\infty}(\Omega)$ is essentially self-adjoint on $L^2(\Omega, dA)$ iff c = 0.

 \rightarrow For c > 0 one should be able to recover the classical limit for certain self-adjoint extensions. "How" is an interesting open question.

 \rightarrow again the compactness hypothesis is not necessary

 \rightarrow For the proof see:

- $c \in [0, 1/2)$ I. Beschastnyi, E. Pozzoli, U. B. Quantum Confinement for the Curvature Laplacian $-\Delta + cK$ on 2D-Almost-Riemannian Manifolds. Potential Theory 2022.
- $c \ge 1/2$, I. Beschastnyi, Closure of the Laplace-Beltrami operator on 2D almost-Riemannian manifolds and semi-Fredholm properties of differential operators on Lie manifolds. arXiv:2104.07745

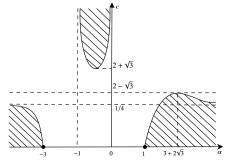
The second case is harder because $-\Delta + cK$ is not "non-negative modulo a Kato small perturbation".

If we remove the 2-step hypotheses the situation could be very different. For instance for the structure

$$X_1=\left(egin{array}{c}1\0\end{array}
ight), \ \ X_2=\left(egin{array}{c}0\x^lpha\end{array}
ight), \ \ lpha\in{f R}$$

(for α integer this structure is almost-Riemannian of step $1 + \alpha$)

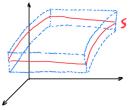
the description of the self-adjointness for $\Delta-cK$ is given by:



the extrinsic approach

Beside geometric quantization, there is a different approach making appearing curvature terms in the operator.

Consider a surface S in \mathbb{R}^3 and let us consider an ε -neighborhood of it.



Let us put boundary conditions (Dirichlet-Dirichlet or Neumann-Neumann) Let us consider the corresponding Laplacians and after a suitable blow up let us send ε to zero. We have:

 $L_{NN}^{\varepsilon} = \Delta + o(\varepsilon)$ $L_{DD}^{\varepsilon} = -\left(\frac{\pi}{2\varepsilon}\right)^{2} + \Delta + (2K - 4H^{2}) + o(\varepsilon)$ (these convergences are weak limits on special test functions) $\rightarrow \text{here } K \text{ is the Gaussian curvature and } H \text{ is the mean curvature}$ $\Rightarrow \text{See Duclos Exper [1995] Lampart Teufel Wachsmuth [2010] filler$

 $\rightarrow \!\!\!$ See Duclos, Exner [1995], Lampart, Teufel, Wachsmuth [2010] for quantum waveguides and Krejcirik [2014].

- For the heat equation only the NN (or periodic) boundary conditions make sense since Dirichlet conditions implies a killing of the process.
- For the Schroedinger equation both boundary conditions make sense (DD after renormalization)
- for the Schroedinger equation other mixed conditions make sense.

Geometric Quantization	extrinsic quantization	
	Δ (Neumann-Neumann)	
$\Delta - cK, c \ge 0$	$\Delta + 2K - 4H^2$ (Dirichlet-Dirichlet)	

Claim Geometric quantization coincides with extrinsic quantization only for c = 0 and for Neumann-Neumann boundary conditions.

can we embed the Grushin Cylinder in ${\bf R}^3$ and compute $\Delta + 2K - 4H^2~?$

 \rightarrow the embedding of the Grushin cylinder can have other applications

The Grushin cylinder is too singular to be embedded globally in \mathbb{R}^3 . However we can embed part of it.

For $x \in [1, \infty[$ and $y \in [0, 2\pi]$ it can be embedded isometrically in \mathbb{R}^3 as

$$z_{1} = const + \int_{1}^{x} \sqrt{1 - \frac{1}{s^{4}}} \, ds, \quad z_{2} = \frac{\cos(y)}{x}, \quad z_{3} = \frac{\sin(y)}{x}, \quad \text{here } (z_{1}, z_{2}, z_{3}) \in \mathbb{R}^{3}$$

(Grushin's trumpet bell)

Claim (expected result): On $[1, \infty[\times S^1, \text{this operator is not essentially self-adjoint.$

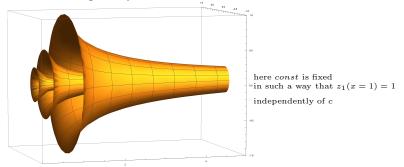
Can we go closer to zero?

If one would like to embed the Grushin cylinder closer to zero up to 1/n one should wind it n^2 times.

More precisely for $x \in [\frac{1}{n}, \infty[$ and $y \in [0, 2\pi]$ we can be embedded isometrically in \mathbb{R}^3 as the surface:

$$z_1 = const + \frac{1}{n} \int_1^{nx} \sqrt{1 - \frac{1}{s^4}} \, ds, \quad z_2 = \frac{\cos(n^2 y)}{n^2 x}, \quad z_3 = \frac{\sin(n^2 y)}{n^2 x}$$

This embedding is only local since the surface is winded n^2 times.



In this case $H = \frac{n^4 x^4 - 3}{2x\sqrt{n^4 x^4 - 1}}$ diverges at $x = \frac{1}{n}$ and $\Delta + 2K - 4H^2$ is not essentially self adjoint in $[\frac{1}{n}, \infty[$.

 \rightarrow it is hard (and not very meaninful) to to say something for $n \rightarrow \infty$.

while for the heat equation the self-adjointness of Δ on $M \setminus Z$ (in the 2-step hypothesis) can be well understood in terms of random walks, for the Schroedinger equations this is harder to be interpreted.

- \rightarrow intrinsic quantizations provides ΔcK which is not self-adjoint except for c = 0.
- \rightarrow extrinsic quantization provides Δ (NN) or $\Delta + 2K 4H^2$ (DD).
 - the first choice coincide with c = 0 of the intrinsic quantization.
 - the second choice cannot be studied at the singularity since the embedding become singular before.

Definition

The Euler number a fully orientable 2D almost-Riemannian structure (\mathbf{U}, f) on a compact manifold M is the Euler number $e(\mathbf{U})$ of \mathbf{U} . It is the self-intersection number of M in \mathbf{U} , where M is identified with the zero section.

we have to specify what we mean by Δ at the singularity \uparrow study the self-adjointness of Δ .

Working with self-adjoint operators is crucial because:

Stone's theorem				
On any Hilbert space there is a one-to-one correspondence,				
A self-adjoint operator	\longleftrightarrow	e^{-itA} strongly continuous unitary group		
Theorem				
On any Hilbert space there is a one-to-one correspondence,				
A nonpositive definite self-adjoint operator	\longleftrightarrow	e^{tA} strongly continuous semigroup		

Let Ω be an open subset of M (possibly coinciding with M).

we recall that an operator $L: D(L) \subset \mathcal{H} \to \mathcal{H}$ is (we assume D(L) dense):

- symmetric if $\langle Lu, v \rangle = \langle u, Lv \rangle$
- self-adjoint if it is symmetric and $D(L^*) = D(L)$

As for the standard Laplacian, Δ is never self-adjoint on $L^2(\Omega, \omega)$ since the domain of Δ^* (that is H^2) is larger than the domain of Δ (e.g., C_c^{∞} , or C_c^2 or $\{\phi \in C^2 \cap L^2 \text{ with } \Delta \phi \in L^2\}$).

Then one defines Δ on $\mathcal{C}^{\infty}_{c}(\Omega)$. We say A is a self-adjoint extension of Δ if

$$D(\overline{\Delta|_{C_c^{\infty}(N)}}) \subset D(A) = D(A^*) \subset D(\Delta^*)$$
$$A^*\phi = \Delta^*\phi \quad \text{for any } \phi \in D(A).$$

We have two cases:

 \rightarrow **There are several self-adjoint extensions.** Each self-adjoint extension corresponds to a different choice of conditions at $\partial\Omega$.

 \rightarrow there exists only one such extension. In this case the operator is called essentially self-adjoint and the extension the Friedrichs extension. Conditions at $\partial\Omega$ are automatically satisfied.

what is important for us is that

- if Δ is essentially self-adjoint then the Cauchy problems for the heat and Schroedinger equations are well posed without the need of boundary conditions
 - for the Schroedinger equation the essential self-adjointness is a necessay and sufficient condition for the well-posedness of the problem
 - for the heat equation it is a sufficient condition