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Quadratic forms, unbounded self-adjoint operators and quantum observables

J. M. Pérez-Pardo(*)
Universidad Carlos III de Madrid - Avd. de la Universidad 30, Leganés, Madrid, Spain

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Summary. — In the context of the geometric formulation of quantum mechanics the observables are characterised by the quadratic forms associated to the self-adjoint operators that describe the corresponding observables in the standard formulation. If the self-adjoint operators are bounded, it can be shown, that their associated quadratic forms are in one-to-one correspondence with the space of real Kählerian functions over the projective Hilbert space defining the system, *i.e.*, over the space of states. However, in the case of unbounded self-adjoint operators such a geometric description is still lacking. The aim of this article is to introduce the main difficulties when dealing with unbounded operators and point out possible generalizations of the geometric notion of observable. In particular, it will be showed how one can work directly with the quadratic forms associated with self-adjoint operators to overcome some of the difficulties. As a motivational example, the case of the Laplace-Beltrami operator is analysed thoroughly.

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1. – Introduction

It is well known that Quantum Mechanics can be treated as an infinite-dimensional Hamiltonian system on a Manifold $\mathcal{PH}$, where $\mathcal{PH}$ denotes the projective Hilbert space associated to the Hilbert space $\mathcal{H}$ (see [1, 2]). In this picture one is provided with the following geometric structures:

– Riemannian metric: $g_{[\Psi]}(\cdot,\cdot)$,
– Symplectic form: $w_{[\Psi]}(\cdot,\cdot)$,
– Complex structure: $J_{[\Psi]}(\cdot)$,

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together with the compatibility conditions

$$g_{[\Psi]}(Ju, Jv) = g_{[\Psi]}(u, v),$$
$$w_{[\Psi]}(u, v) = g_{[\Psi]}(Ju, v),$$

where $[\Psi]$ stands for a generic element of $\mathcal{PH}$ and $u, v \in T_{[\Psi]}\mathcal{PH}$. In other words, the quantum system has the structure of a Kähler manifold. Any physically relevant quantity can be obtained directly in terms of these structures. For instance, the transition probability between two states $|\langle \Psi \,, \Phi \rangle|^2$ is directly related to the geodesic distance between the two points $[\Phi]$ and $[\Psi]$. Commutation relations are given by the symplectic structure and the Riemannian metric measures the dispersion of the observables. In every Kähler manifold there is a special class of functions that can be defined, namely the Kählerian functions. A Kählerian function is a *smooth* function over the manifold $f \in \mathcal{C}^\infty(\mathcal{PH}, \mathbb{C})$ such that its associated Hamiltonian vector field X_f, defined by $w(X_f, \cdot) = \mathrm{d}f(\cdot)$, is also a Killing field. Kählerian functions are therefore those functions whose associated Hamiltonian vector fields preserve simultaneously both, the symplectic structure and the Riemannian structure, *i.e.*,

$$\mathcal{L}_{X_f} w = 0,$$
$$\mathcal{L}_{X_f} g = 0.$$

It can be proved [2] that any *smooth* real Kählerian function $f \in \mathcal{C}^\infty(\mathcal{PH}, \mathbb{R})$ is in correspondence with a linear *bounded* self-adjoint operator A acting on $\mathcal{H}$, the correspondence being explicitly given by

$$f([\Psi]) = \frac{\langle \Psi \,, A\Psi \rangle}{\|\Psi\|^2} \,.$$

Thus, Kählerian functions are precisely the observable quantities associated to the bounded self-adjoint operators. It seems therefore that the geometrical picture is complete, because any meaningful quantity can be recovered just from the corresponding geometrical objects in the picture. Unfortunately, this is only true for finite dimensional systems, where any observable is given by a bounded self-adjoint operator. In the infinite-dimensional situation one has to deal with unbounded operators. In fact, the most important examples are of this later kind, like the angular momentum, the linear momentum or the kinetic energy, just to mention a few.

The main problem when trying to define observables in the generic infinite dimensional situation is that unbounded operators are not continuous, thus complicating the task of relating them with intrinsic geometric objects. It is worth to mention that the difficulties arising when dealing with unbounded operators are not exclusive from the geometric picture. For example, in the C^*-algebraic approach to quantum physics one needs to work with bounded operators and one way to overcome the difficulty in that case is to go through the one-parameter unitary groups that are associated to any self-adjoint operator (cf. [2, 3] and references therein). One possibility in order to obtain possible generalizations of the geometric notion of observable is to restore the continuity. For instance, self-adjoint operators are closed. This property allows to define some subspaces of $\mathcal{H}$, where continuity is not completely lost. In sect. **2** unbounded symmetric operators are briefly introduced together with the main difficulties associated to them. The theory of representations of quadratic forms is presented also in this section and other possible definitions of the notion of observable are suggested inspired on these results. Section **3** is devoted to analyse the particular example of the Laplace-Beltrami operator on a compact Riemannian manifold.

2. – Unbounded self-adjoint operators and quadratic forms

We begin reviewing standard material. See [4] for details and proofs. In what follows we are going to consider linear operators T acting on the Hilbert space $\mathcal{H}$. The standard notations $\langle\cdot\,,\cdot\rangle$ and $\|\cdot\|$ will be used for the scalar product and the norm in $\mathcal{H}$, respectively. The operator T is going to be defined on a domain $\mathcal{D}(T)$,

$$T : \mathcal{D}(T) \to \mathcal{H}.$$

The domain $\mathcal{D}(T)$ is assumed to be dense in $\mathcal{H}$, $\overline{\mathcal{D}(T)}^{\|\cdot\|} = \mathcal{H}$. An operator is said to be bounded if there exists a constant M such that

$$\|T\Phi\| \leq M\|\Phi\|, \quad \forall\ \Phi \in \mathcal{D}(T).$$

Notice that this condition for a linear operator is exactly the condition for continuity,

$$\|T\Phi - T\Phi'\| = \|T(\Phi - \Phi')\| \leq M\|\Phi - \Phi'\|. \tag{1}$$

Hence, in the bounded case, even if the operator is defined only in the dense subspace $\mathcal{D}(T)$, it can be extended to the whole Hilbert space. Let $\Phi_n \to \Phi$. Then, because of eq. (1), $T\Phi_n$ is a Cauchy sequence too and its limit exists. Then, one can define

$$T\Phi := \lim_{n\to\infty} T\Phi_n.$$

In general, one does not need to define a domain for a bounded operator because it is defined in the whole Hilbert space. On the contrary, for unbounded operators, a domain must be specified. Consider for instance the linear momentum operator $T = i\frac{\mathrm{d}}{\mathrm{d}x}$ acting on the Hilbert space $\mathcal{H} = \mathcal{L}^2[0,1]$. It is clear that $\sqrt{x} \in \mathcal{L}^2[0,1]$ but $T(\sqrt{x}) = i\frac{1}{2\sqrt{x}} \notin \mathcal{L}^2[0,1]$. Moreover, even if one is able to select a dense domain $\mathcal{D}(T)$ for T such that

$$\|T\Phi\| < \infty, \quad \forall\ \Phi \in \mathcal{D}(T)$$

one can not extend this operator to the whole Hilbert space. This is so because for unbounded operators there will always exist elements $\Phi \in \mathcal{H}$ such that the image under T of any sequence $\Phi_n \in \mathcal{D}(T)$ converging to them will necessarily diverge, *i.e.*,

$$\|T\Phi_n\| \to \infty, \quad \Phi_n \in \mathcal{D}(T).$$

The way to handle this difficulty is to introduce the notion of *closed* operators. A linear operator is said to be closed if given a Cauchy sequence $\Phi_n \in \mathcal{D}(T)$ such that $T\Phi_n \in \mathcal{H}$ is also a Cauchy sequence, implies that $\Phi \in \mathcal{D}(T)$ and that $\lim T\Phi_n = T\Phi$. So, even if closed operators might not be continuous, they are continuous on their domains. A useful characterization is given by introducing the *graph-norm* of the operator T,

$$|||\cdot||| := \sqrt{\|\cdot\|^2 + \|T\cdot\|^2}.$$

An operator is closed if and only if its domain is closed with respect to this norm,

$$\overline{\mathcal{D}(T)}^{|||\cdot|||} = \mathcal{D}(T).$$

In the same way that we can extend a bounded operator from a dense domain to the whole Hilbert space, we can try to extend an operator that is not closed to a domain where it is closed. We will say that the operator $\tilde{T}$ *extends* T and denote it like $T \subset \tilde{T}$ if $\mathcal{D}(T) \subset \mathcal{D}(\tilde{T})$ and $\tilde{T}\big|_{\mathcal{D}(T)} = T$. An operator is said to be *closable* if it has closed extensions. Unbounded operators do not need to be closable, however there is an important class of operators, the symmetric operators, for which closed extensions always exist. An operator T is said to be symmetric if

$$\langle \Phi\,, T\Psi \rangle = \langle T\Phi\,, \Psi \rangle, \quad \forall\; \Phi, \Psi \in \mathcal{D}(T).$$

This means that the adjoint operator $T^\dagger$ extends T, *i.e.*,

$$T \subset T^\dagger.$$

The adjoint operator is always a closed operator and therefore symmetric operators are always closable. An operator is said to be *self-adjoint* when $T = T^\dagger$. It is worth to say that if the operators are bounded, the notions of symmetric and self-adjoint operators coincide. The nice properties associated in linear algebra for Hermitean matrices have their analogs only for self-adjoint operators. For instance, any self-adjoint operator has real spectrum. Symmetric operators that are not self-adjoint have as spectrum either the full complex plane, the upper complex half-plane or the lower complex half-plane. Self-adjoint operators admit an integral representation, known as the spectral theorem, which coincides with the expansion of the operator in the orthonormal projectors associated to its eigenvalues when the spectrum is discrete. We can write

$$T = \int_\sigma \lambda \mathrm{d}E(\lambda) = \sum_\alpha \lambda_\alpha P_\alpha,$$

where the last inequality holds only if the spectrum of T, σ, is discrete. Another property that is characteristic for self-adjoint operators is that Stone's Theorem relates them with strongly continuous one-parameter unitary groups. An operator T is the generator of a one-parameter unitary group, U_t, if and only if T is a self-adjoint operator and then

$$U_t\Phi = e^{itT}\Phi. \tag{2}$$

In general it is easy to construct closed symmetric operators. One needs to find an operator that is symmetric, like the momentum operator $T = i\frac{\mathrm{d}}{\mathrm{d}x}$ above, and close it. That means that one can extend the operator to a domain where it is closed. The easiest way is to take the domain that is the closure in the graph norm of the domain of the symmetric operator, *i.e.*, to consider the operator defined on the domain

$$\overline{D(T)}^{|||\cdot|||}.$$

For symmetric operators one can always obtain a closed extension by doing so. The problem is that such extension is not self-adjoint in general. Symmetric operators may have no self-adjoint extensions. For example, the momentum operator on the half-line has none. In general, even if a self-adjoint extension exists, it may be non-unique. As an example of this latter situation one can take the Laplace operator defined on an interval I. It is well known that fixing the boundary conditions is a good way to characterise different self-adjoint extensions of differential operators. Both, the Laplace operator with Dirichlet boundary conditions and the Laplace operator with periodic boundary conditions determine two different but physically meaningful self-adjoint extensions of the symmetric Laplace operator Δ defined on the smooth functions with compact support in the interior of the interval $\mathcal{D}(\Delta) = \mathcal{C}^\infty_c(I)$.

It is worth noticing that, even if the generator is an unbounded operator, the one-parameter group generated by it is always a bounded operator and is therefore continuous. Moreover, any linear continuous operator acting on a Hilbert space is infinitely differentiable because the second derivative is the zero operator(1) (see [5] for details on derivatives of operators between Banach spaces). This motivates the following definition taken from [6]. A *Kähler isomorphism* is a smooth diffeomorphism $\Theta : \mathcal{PH} \to \mathcal{PH}$, such that

$$\Theta^* w = w,$$
$$\Theta^* g = g.$$

Stone's Theorem guaranties that any self-adjoint operator T (not necessarily bounded) defines a strongly continuous one-parameter group of Kähler isomorphisms

$$\Theta_t([\Psi]) := \exp(itT)[\Psi].$$

Notice that this isomorphisms are smooth for every value of t. The boundedness of the operator T amounts for the infinite differentiability with respect to the parameter t. One can therefore define the quantum observables to be the generators of the one-parameter groups of Kähler isomorphisms. Doing this, however, does not solve the problem of the non-uniqueness of self-adjoint extension for symmetric operators. All the self-adjoint extensions of a given symmetric operator would be admitted observables at the same time. For instance, considering the example of the Laplace operator above, with Dirichlet and periodic boundary conditions, both self-adjoint extensions define the energy of the system but in two different dynamical situations. It does not seem to be reasonable to have both of them to be observables at the same time. A way to avoid this situation is to select a proper dense subspace where all the observables can be defined at the same time and that can be extended by continuity to the corresponding closed extensions. Clearly, selecting domains were the operators are just symmetric is not a good strategy because this does not lead to unambiguously defined self-adjoint extensions.

(1) It is obviously not infinitely differentiable with respect to the parameter t.

Fortunately, there are other objects that can also be related naturally to the quantum observables and that could address this problem, the quadratic forms. To each self-adjoint operator T one can associate a quadratic form Q_T using the spectral resolution of the identity E_λ provided by the spectral theorem. One defines the domain of the quadratic form as

$$\mathcal{D}(Q_T) := \left\{ \Phi \in \mathcal{H} \;\Big|\; \int_{\sigma(T)} |\lambda| \mathrm{d}\langle \Phi \,, E_\lambda \Phi \rangle < \infty \right\}, \tag{3}$$

and the quadratic form is then simply

$$Q_T(\Phi, \Psi) := \int_{\sigma(T)} \lambda \mathrm{d}\langle \Phi \,, E_\lambda \Psi \rangle, \tag{4}$$

which is precisely the expectation value function associated to T if $\Psi \in \mathcal{D}(t)$, *i.e.*, $Q_T(\Phi, \Psi) = \langle \Phi \,, T\Psi \rangle$. In general, however, the domain of the quadratic form is bigger than the domain of the associated operator. This means that even though both objects are intimately related, they do not have the same continuity properties when considered as objects defined on the Hilbert space $\mathcal{H}$. In fact, one can consider a quadratic form as a Hermitean sesquilinear form $Q(\Phi, \Psi) = \overline{Q(\Psi, \Phi)}$ defined on the Hilbert space and, under some extra assumptions shown below, it can be proved that this quadratic form is the quadratic form associated to a *unique* self-adjoint operator. We will consider from now on just lower semibounded quadratic forms. A quadratic form is lower semibounded if there exists a constant $M > 0$ such that $Q(\cdot, \cdot) \geq -M\| \cdot \|^2$. In the same way that unbounded operators, quadratic forms do not need to be defined on the whole Hilbert space but can satisfy a weaker notion of continuity. A lower semibounded quadratic form is said to be *closed* if $\mathcal{D}(Q)$ is complete with respect to the graph norm of that quadratic form defined by

$$\|\!| \cdot |\!\|_Q := \sqrt{(M+1)\| \cdot \|^2 + Q(\cdot\,, \cdot)}.$$

The semiboundedness assumption is crucial for this expression to define a norm. Then, it can be proved the following (cf. [7,8]):

Theorem 1. Let $Q\colon \mathcal{H} \to \mathbb{R}$ be a lower semibounded quadratic form. The following statements are equivalent:

- *Q is the quadratic form associated to a lower semibounded self-adjoint operator.*
- *Q is a lower semicontinuous function, i.e.,*

$$\liminf_{n\to\infty} Q(\Phi_n) \geq Q(\Phi).$$

- *The domain $\mathcal{D}$ of the quadratic form is complete with respect to the graph-norm $\|\!| \cdot |\!\|_Q$.*

This theorem assures that to every semibounded quadratic form whose domain is complete with respect to the graph-norm it exists a self-adjoint operator such that the quadratic form can be expressed as in eqs. (3) and (4). In the same way that one can have closable operators, one can have closable quadratic forms. A quadratic form

TABLE I. – *Differences between closable operators and closable quadratic forms.*

Closable Operators	Closable Quadratic Forms
Symmetric operators are always closable.	Hermitean q.f. are *not* always closable.
The minimal extension is *not* necessarily s.a..	The minimal extension is s.a. (Friedrichs' extension).

is said to be *closable* if it possesses closed extensions. The remarkable fact is that for every closed extension there exists a unique self-adjoint operator. Thus, the quadratic forms provide a nice way to construct self-adjoint extensions of symmetric operators. Moreover, there is one preferred closed extension which is the quadratic form associated to the closure of the domain. This closed extension is known as *Friedrichs' extension* and is always associated to a self-adjoint operator due to the previous theorem. It is worth to point out the differences between closable operators and closable forms. The adjoint of a symmetric operator is densely defined and this is a sufficient condition for an operator to be closable. Thus, symmetric operators are always closable and one can consider their minimal closed extension. When the minimal extension of a symmetric operator is a self-adjoint operator, the operator is said to be *essentially self-adjoint*. However, the minimal extension is in general not a self-adjoint operator. Moreover, it may happen that any of the closed extensions define a self-adjoint operator. On the contrary, Hermitean quadratic forms are not always closable. Take as an example the quadratic form $Q(\Phi) := |\Phi(0)|^2$ defined on $\mathcal{C}^\infty(\mathbb{R}) \subset \mathcal{L}^2(\mathbb{R})$. However, if the quadratic form is closable, the minimal extension is associated to a unique self-adjoint operator. The main differences are summarised in table I.

Inspired in the statement of the theorem one can therefore define the quantum observables in the geometric picture of quantum mechanics to be those lower semibounded functions on $\mathcal{PH}$ that are real and lower semicontinuous. Of course, this definition is not completely satisfactory because there are self-adjoint operators that are not lower semibounded. A great step in the direction of finding a proper definition of quantum observables in the geometric picture would be to obtain a generalization of the representation theorem above that works with general self-adjoint operators, not just with semibounded ones.

3. – Example: the Laplace-Beltrami operator on a compact Riemannian manifold

In this section we will work out explicitly the example of the Laplace-Beltrami operator from the point of view of the quadratic forms. This operator defines the dynamics of a free particle constrained to a Riemannian manifold Ω, the Hilbert space of the system being $\mathcal{H} = \mathcal{L}^2(\Omega)$. The self-adjoint extensions of this operator are well known [9], especially in the 1 dimensional case. The Laplace-Beltrami operator on a compact Riemannian manifold (Ω, η) is given by

$$\Delta_\eta := \sum_{j,k} \frac{1}{\sqrt{|\eta|}} \frac{\partial}{\partial x^j} \sqrt{|\eta|}\eta^{jk} \frac{\partial}{\partial x^k} .$$

Now, taking $\Phi \in \mathcal{C}^\infty(\Omega)$ one can define

$$Q(\Phi) := \langle \mathrm{d}\Phi \,, \mathrm{d}\Phi\rangle - \langle \varphi \,, \dot{\varphi}\rangle_{\mathcal{L}^2(\partial\Omega)}, \tag{5}$$

where the definition comes from integrating by parts the expression $\langle \Phi \,, -\Delta_\eta \Phi\rangle$ once. We denote by $\varphi = \Phi|_{\partial\Omega}$ and $\dot{\varphi} = \partial\Phi/\partial\mathbf{n}|_{\partial\Omega}$, respectively, the restriction to the boundary and the restriction of the normal derivative pointing outwards to the boundary. The second term above, $\langle \cdot \,, \cdot\rangle_{\partial\Omega}$, stands for the induced scalar product at the boundary. The quadratic form (5) is not an Hermitean quadratic form because

$$\langle \varphi \,, \dot{\varphi}\rangle_{\mathcal{L}^2(\partial\Omega)} \neq \langle \dot{\varphi} \,, \varphi\rangle_{\mathcal{L}^2(\partial\Omega)}.$$

It would be Hermitian if we were able to find domains that are maximally isotropic subspaces of the sesquilinear form

$$\Sigma(\Phi, \Psi) := \langle \varphi \,, \dot{\psi}\rangle_{\mathcal{L}^2(\partial\Omega)} - \langle \dot{\varphi} \,, \psi\rangle_{\mathcal{L}^2(\partial\Omega)}. \tag{6}$$

From now on, the subscript on the induced scalar product at the boundary will be understood. It is also well known (see for instance [10]) that maximally isotropic subspaces of this sesquilinear form are in one-to-one correspondence with unitary operators acting on the Hilbert space of the boundary $U \in \mathcal{U}(\mathcal{L}^2(\partial\Omega))$. This correspondence is explicitly given by the following transformation of the boundary data (Cayley transform) $\varphi_\pm = \varphi \pm i\dot{\varphi}$. With this transformation the boundary form in eq. (6) becomes

$$\tilde{\Sigma}(\Phi, \Psi) := i\big[\langle \varphi_+ \,, \psi_+\rangle - \langle \varphi_- \,, \psi_-\rangle\big], \tag{7}$$

showing clearly that functions satisfying $\varphi_- = U\varphi_+$ make the boundary form vanish identically. Undoing the Cayley transform we get the desired boundary conditions as introduced in [11]

$$\varphi - i\dot{\varphi} = U(\varphi + i\dot{\varphi}). \tag{8}$$

For each unitary U we can therefore define a domain where the quadratic form is Hermitean and that we shall denote

$$\mathcal{D}_U = \big\{\Phi \in \mathcal{C}^\infty(\Omega) \mid \varphi - i\dot{\varphi} = U(\varphi + i\dot{\varphi})\big\}. \tag{9}$$

Strictly speaking one needs to be careful in dimension higher than 1 because the space of boundary data $(\varphi, \dot{\varphi})$ is not the complete space $\mathcal{L}^2(\partial\Omega) \times \mathcal{L}^2(\partial\Omega)$ but a more regular subset of it involving Sobolev spaces. There are ways to handle this situation with greater generality but they are outside the scope of this article and will be treated elsewhere (see [12] for more details). In order to keep the discussion simple, it is enough to assume that the unitary operator defining the boundary condition preserves the space of smooth functions at the boundary.

As should be clear from the discussion in the previous section we need the quadratic form to be semibounded. We need to impose extra conditions on the unitary U defining the Hermitean domain. We will say that the unitary has *gap* κ if in the intersection between a ball of radius κ centred in -1 and the spectrum of the unitary operator U there is at most the eigenvalue -1. It is clear that the first term in eq. (5) is positive, so that we need to find a bound for the boundary term. We can use the spectral theorem for unitary operators to split the Hilbert space at the boundary into two closed subspaces, namely, the closed eigenspace $\mathcal{W}$ associated to -1 and its orthogonal complement $\mathcal{W}^\top$. The boundary condition can then be rewritten using this splitting

$$\varphi_{\mathcal{W}} - i\dot{\varphi}_{\mathcal{W}} = U_{\mathcal{W}}(\varphi_{\mathcal{W}} + i\dot{\varphi}_{\mathcal{W}}) \Rightarrow \varphi_{\mathcal{W}} = 0$$
$$\varphi_{\mathcal{W}^\top} - i\dot{\varphi}_{\mathcal{W}^\top} = U_{\mathcal{W}^\top}(\varphi_{\mathcal{W}^\top} + i\dot{\varphi}_{\mathcal{W}^\top}) \Rightarrow \dot{\varphi}_{\mathcal{W}^\top} = i\frac{U_{\mathcal{W}^\top} - \mathbb{I}}{U_{\mathcal{W}^\top} + \mathbb{I}}\varphi_{\mathcal{W}^\top} := A_{\mathcal{W}^\top}\varphi_{\mathcal{W}^\top}\,.$$

The last implication follows from the gap condition on U which makes the operator $A_{\mathcal{W}^\top}$ bounded. We can now write the boundary term using this decomposition

$$\text{(10)}\quad \langle\varphi\,,\dot{\varphi}\rangle = \langle\varphi_{\mathcal{W}}\,,\dot{\varphi}_{\mathcal{W}}\rangle + \langle\varphi_{\mathcal{W}^\top}\,,\dot{\varphi}_{\mathcal{W}^\top}\rangle \leq \|A_{\mathcal{W}^\top}\|\|\varphi_{\mathcal{W}^\top}\|^2 \leq \|A_{\mathcal{W}^\top}\|\|\varphi\|^2 \leq C\|A_{\mathcal{W}^\top}\|\|\Phi\|^2_{\mathcal{H}^1}\,.$$

The last inequality is a direct application of the Lion trace inequalities, cf. [13], from which $\|\varphi\|^2 \leq C\|\Phi\|^2_{\mathcal{H}^1}$ is an immediate consequence and $\|\cdot\|_{\mathcal{H}^1}$ stands for the norm of the Sobolev space of order 1 on the Riemannian manifold Ω. This shows that $|Q(\Phi)| \leq C'\|\Phi\|^2_{\mathcal{H}^1}$ if the elements in the domain verify eq. (8), which guaranties that the quadratic form is closable, according to [8]. If the quadratic form is lower semibounded then Thm. 1 assures that the quadratic form is related with a self-adjoint operator. It is an easy calculation to show that if the factors in the last inequality above verify $C\|A_{\mathcal{W}^\top}\| < 1$, then the quadratic form is semibounded with the same constant. So far we have proved that the quadratic forms eq. (5) with domains eq. (9) are closable provided that the unitary has gap and that the gap is big enough, because in that case $\|A_{\mathcal{W}^\top}\|$ can be as small as needed. Simple integration by parts in eq. (5) shows that the self-adjoint operator corresponds to a self-adjoint extension of the Laplace-Beltrami operator.

Using the quadratic form approach we have been able to characterise a wide class of self-adjoint extensions of the Laplace-Beltrami operator that are lower semibounded. Belonging to this class are the well known Dirichlet and Neumann boundary conditions, that correspond to $U = -\mathbb{I}$ and $U = \mathbb{I}$, respectively, but clearly there are many others.

4. – Conclusions

Quadratic forms arise as the natural objects to define observables in quantum mechanics, not just in the geometric picture. It is still an open problem to identify the necessary conditions for a generic unbounded quadratic form to be representable as in eq. (4). It is needless to say that such a result would have deep implications in quantum mechanics, not just in the formalization of the geometric picture, and in other fields like functional analysis or numerical analysis because quadratic forms are objects that are intimately related with the operators that define them. In fact, they contain information about the spectrum of the operator (min-max Principle) and, because they are explicitly Hermitean, they are more suitable for numerics.

The example in sect. **3** is treated with greater generality in a joint work with A. Ibort and F. Lledó (to appear soon). In particular, all the conditions on U can be removed except the gap condition showing that, for the Laplace-Beltrami operator, the quadratic forms introduced in the previous section are representable even if they are not semibounded. The author hopes that this example points out proper conditions for a generic quadratic form to be representable in terms of a self-adjoint operator and, incidentally, be the guide for a better description of the observables in quantum mechanics.

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