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Finite element method to solve the spectral problem for arbitrary self-adjoint extensions of the Laplace–Beltrami operator on manifolds with a boundary [☆]

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ABSTRACT

A numerical scheme to compute the spectrum of a large class of self-adjoint extensions of the Laplace–Beltrami operator on manifolds with boundary in any dimension is presented. The algorithm is based on the characterisation of a large class of self-adjoint extensions of Laplace–Beltrami operators in terms of their associated quadratic forms. The convergence of the scheme is proved. A two-dimensional version of the algorithm is implemented effectively and several numerical examples are computed showing that the algorithm treats in a unified way a wide variety of boundary conditions.

1. Introduction

The study of self-adjoint extensions of symmetric operators plays a fundamental role not only in the foundations, but increasingly so in the applications of Quantum Mechanics as they determine the spectrum of the corresponding system. Among them, it is paramount the role played by the Laplace–Beltrami operator, as it corresponds to the to the time independent Schrödinger equation for a free particle.

When boundaries are present such operators can be defined easily on a domain where it is symmetric but usually not self-adjoint. Self-adjointness is a crucial property that guarantees the reality of the spectrum. Moreover, Stone's Theorem establishes that it also guarantees the unitarity of the evolution governed by the Schrödinger equation. See, e.g. [44, Chapter X] for further details and motivation. Starting from a symmetric operator one needs to choose a self-adjoint extension of it, which in general is not unique. In the present context of differential operators on manifolds with boundaries this is done by selecting appropriately boundary conditions. Different boundary conditions represent different physical situations, see for instance the reviews [6,30] and references therein. Consider the Laplace operator on an interval. Dirichlet boundary conditions represent a particle trapped in a box while quasiperiodic boundary conditions represent that the particle is mov-

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ing on a closed curve surrounding a magnetic field [5]. Other boundary conditions represent other physical situations. For instance, they can be chosen to represent point like interactions [19].

In dimension one, the problem of characterising self-adjoint extensions and computing their spectrum and eigenvectors was addressed in [29]. However, the algorithm proposed there cannot be applied in dimension higher than one in a straightforward way. The main reason for this is that in dimension higher than one the space of self-adjoint extensions is infinite dimensional [23,27]. In dimension one, the self-adjoint extensions can be parameterised by the set of unitary operators acting on a finite dimensional vector space and therefore they can be implemented exactly. This is not the case in dimension higher than one where in general one needs also to approximate the boundary conditions. This needs to be handled carefully when proving the convergence of a numerical scheme approximating the spectrum. The numerical study of self-adjoint extensions for the Laplace–Beltrami operator in dimension higher than one is also interesting from a mathematical perspective since it requires the development of finite element methods (FEM) that use completely different constructions of boundary elements than for the already well developed Dirichlet and Neumann boundary conditions, cf. [8,13,42].

New quantum technologies and applications require the implementation of boundary conditions that go beyond the usual ones in order to have a good description of their properties. For instance, Quantum Hall effect [36,12], superconductors surrounded by insulators [3,4], Casimir Effect [41,34,2], computation of solutions of Bloch periodic wave-functions on periodic lattices [47] and other novel proposals like the generation of entanglement or the study of topology change by modifying the boundary conditions [28,40]. Self-adjoint boundary conditions can also be used to model physical situations like point interactions [19] or resonators coupled to thin antennas [15,21,22]. It is important to notice that the addition of regular potentials does not jeopardise the self-adjointness of the domain of a differential operator, cf. [44,31]. Hence, the analysis carried out in this article can be used straightforwardly for Schrödinger operators by just computing the contribution of the potential as it is done in standard FEM.

In this context, boundary conditions are going to be treated as the only input parameter of the problem and the geometry will remain fixed. In the standard FEM approach, one needs to distinguish *a priori* which boundary conditions are essential and which ones are natural in order to construct the appropriate FEM. In contrast, the algorithm presented here treats natural and essential boundary conditions in a unified way. It is able to deal with a diversity of boundary conditions like Dirichlet, Neumann, Robin, mixed, periodic, quasi-periodic (also called Bloch-periodic), or even more general ones like those appearing in [26] by just modifying the input parameters.

This article focuses on the construction and analysis of the aforementioned algorithm to show its capabilities. Moreover, the convergence conditions of this approach are proven not only for the particular realisation presented here, but for a general situation. The approach for the construction of finite elements at the boundary, as it is proposed here, should be taken as a complement to already existent and well-established all-purpose routines, for instance, the one presented in [46]. However, standard approaches do not allow to solve the problem for the variety of boundary conditions that can be handled with the present scheme. Implementation of more efficient approaches to speed up convergence will be considered in the future. These include mesh refinements or increasing the polynomial degree of the finite elements, i.e. implementation of h-method or p-method, as well as other recent developments like including probabilistic indetermination of the input data as it is done in [7,10,11]. These latter considerations will play a relevant role when considering more complex geometries than the ones considered here.

The implementation of the FEM to cope with boundary conditions defined by unitary operators at the boundary is performed by adding a rim of boundary elements to the domain that serve to implement the finite dimensional approximation of the domain of the given operator. Such elements have a particular structure that has been carefully crafted to guarantee the convergence of the domains and the quadratic forms approximating the original problem. In order to implement all these different boundary conditions it is only needed to add the aforementioned rim of boundary elements. In the interior of the domain, the bulk, one can use well developed numerical schemes that are already available, for instance [46].

The article is organised as follows. In Section 2 we introduce the family of self-adjoint extensions of the Laplace–Beltrami operator that is suitable for the numerical approximation of its spectrum. In Section 3 we provide sufficient conditions on the approximants of the spectral problem to guarantee convergence to the exact solutions and in Section 4 we construct them explicitly. In order to test the performance of the scheme we have built a standard finite element method at the bulk and we have complemented it with the proposed construction at the boundary. In Section 5 several numerical experiments with applications in Physics have been solved to show the capabilities of the proposed scheme. The pseudocode of the implementation can be found in the appendix.

2. Self-adjoint extensions of the Laplace–Beltrami operator and unitary operators at the boundary

In this section we introduce the family of operators that will be addressed by the numerical algorithm. We will present the most important results in order to keep the article as self-contained as possible. This will also serve to fix the notation.

Let $(\Omega, \partial\Omega, \eta)$ be a smooth orientable Riemannian manifold with metric η and smooth compact boundary $\partial\Omega$. We will denote as $\mathcal{C}^\infty(\Omega)$ the space of smooth functions on the Riemannian manifold Ω, and by $\mathcal{C}_c^\infty(\Omega)$ the space of smooth functions with compact support in the interior of Ω. The Riemannian volume form is denoted by $\mathrm{d}\mu_\eta$.

The **Laplace–Beltrami Operator** associated to the Riemannian manifold $(\Omega, \partial\Omega, \eta)$ is the second order differential operator $\Delta_\eta : \mathcal{C}^\infty(\Omega) \to \mathcal{C}^\infty(\Omega)$ given in local coordinates (x^i) on Ω by