

## ANISOTROPIC GRADED MESHES AND QUASI-OPTIMAL RATES OF CONVERGENCE FOR THE FEM ON POLYHEDRAL DOMAINS IN 3D

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**Abstract.** We consider the model problem  $-\Delta u + Vu = f \in \Omega$ , with suitable boundary conditions on  $\partial\Omega$ , where  $\Omega$  is a bounded polyhedral domain in  $\mathbb{R}^d$ ,  $d = 2, 3$ , and  $V$  is a possibly singular potential. We study efficient finite element discretizations of our problem following Numer. Funct. Anal. Optim., 28(7-8):775–824, 2007, Bull. Math. Soc. Sci. Math. Roumanie (N.S.), 55(103):157–178, 2012, and a few other more recent papers. Under some additional mild assumptions, we show how to construct sequences of meshes such that the sequence of Galerkin approximations  $u_k \in S_k$  achieve  $h^m$ -quasi-optimal rates of convergence in the sense that  $\|u - u_k\|_{H^1(\Omega)} \leq C \dim(S_k)^{-m/d} \|f\|_{H^{m-1}(\Omega)}$ . Our meshes defining the Finite Element spaces  $S_k$  are suitably graded towards the singularities. They are topologically equivalent to the meshes obtained by uniform refinement and hence their construction is easy to implement. We explain in detail the mesh refinement for four typical problems: for mixed boundary value/transmission problems for which  $V = 0$ , for Schrödinger type operators with an inverse square potential  $V$  on a polygonal domain in 2D, for Schrödinger type operators with a periodic inverse square potential  $V$  in 3D, and for the Poisson problem on a three dimensional domain. These problems are listed in the increasing order of complexity. The transmission problems considered here include the cases of multiple junction points.

## Introduction

Let  $\Omega \subset \mathbb{R}^d$  be an open, bounded set. Consider the model problem

$$(-\Delta + V)u = f \text{ in } \Omega \quad (1)$$

defined on a bounded domain  $\Omega \subset \mathbb{R}^d$ , where  $\Delta$  is the Laplacian  $\Delta = \sum_{i=1}^d \partial_i^2$ . Suitable boundary conditions will be imposed. This model problem (even for  $V = 0$ ) arises in many practical applications. We are interested in finding efficient numerical methods for the approximation of the solution  $u$ . In this paper we shall deal with the classical Finite Element Method. The rate of convergence of the Finite Element approximations  $u_k$  of  $u$  depends (at least for quasi-uniform meshes) on the smoothness of the solution  $u$ .

When  $\partial\Omega$  is smooth and  $V = 0$ , it is well known that our model problem (1) has a unique solution  $u \in H^{m+1}(\Omega)$  for any  $f \in H^{m-1}(\Omega)$  and  $g \in H^{m+1/2}(\partial\Omega)$  [6], where  $g$  is the Dirichlet boundary condition,  $u = g$  on  $\partial\Omega$ . Moreover,  $u$  depends continuously on  $f$  and  $g$ . This result is the *classical well-posedness of the Poisson problem* on smooth domains and provides a satisfactory smoothness result for  $u$ . On the other hand, when  $\Omega$  is not smooth and  $V = 0$ , it is also well known [4, 5, 9, 10, 11] that there exists  $s = s_\Omega$  such that  $u \in H^s(\Omega)$  for any  $s < s_\Omega$ . Nevertheless,  $u \notin H^{s_\Omega}(\Omega)$  in general, even when  $f$  and  $g$  are smooth functions, and this does affect the rates of convergence of the Finite Element approximations.

In what follows, we shall fix  $m \geq 1$ . The parameter  $m$  denotes the desired rate of convergence in the Finite Element Method. Let us consider a sequence of finite dimensional subspaces  $S_k \subset H^1(\Omega)$  and denote by  $u_k \in S_k$  the Galerkin finite element projections of the solution  $u$  of Equation (1) for  $f \in H^{m-1}(\Omega)$ . We assume that the sequence  $S_k$  satisfies all essential boundary conditions imposed on our problem. Then we shall say that our sequence  $u_k$  achieves  *$h^m$ -quasi-optimal rates of convergence* if there exists a constant  $C > 0$ , independent of  $k$  and  $f$ , such that

$$\|u - u_k\|_{H^1(\Omega)} \leq C \dim(S_k)^{-m/d} \|f\|_{H^{m-1}(\Omega)}, \quad u_k \in S_k, \quad (2)$$

where  $d = 2$  or  $d = 3$  is the dimension of our polyhedral domain  $\Omega$ . The amount of work required to find  $u_k$  depends on the dimension of  $S_k$ , so it is natural to compare the error with  $\dim(S_k)$ , especially since the usual parameter  $h$  loses its meaning for a non quasi-uniform sequence of meshes. Our main goal is to define suitable subspaces  $S_k \subset H^1(\Omega)$ , satisfying all essential boundary conditions in our problem, such that the Galerkin finite element projections  $u_k \in S_k$  that approximate the solution  $u$  of Equation (1) for  $f \in H^{m-1}(\Omega)$  achieve  *$h^m$ -quasi-optimal rates of convergence*. We shall show how this is done in the four cases mentioned in the abstract:

- 1) for mixed boundary value/transmission problems with  $V = 0$  in 2D,
- 2) for Schrödinger type operators with inverse square potential  $V$  on a polygonal domain in 2D,
- 3) for Schrödinger type operators with a periodic inverse square potential  $V$  in 3D, and
- 4) for the Poisson problem (so  $V = 0$ ) on a three dimensional domain.

The above cases were listed in the increasing order of complexity. The transmission problems considered here in 2D include the cases of multiple junction points.

The rest of the paper is organized as follows. In the first section, we review well posedness results for transmission problems in isotropic weighted Sobolev spaces, and present a new well-posedness result for interface problems in 2D with  $V \neq 0$  singular. The quasi-optimal mesh refinement strategy for our 2D problem is presented in Section 2. The refinement used in 2D is the same type of refinement as the one used for the faces of our meshes in 3D. In Section 3, we discuss the case of a Schrödinger operator with an inverse square potentials the 3D case. In the last section (Section 4) we describe the construction of sequences of meshes that yields  $h^m$ -quasi-optimal rates of convergence for the Poisson problem on a three dimensional polyhedral domain. This refining procedure extends (and builds on) the refinement procedure in Section 3. From the point of view of implementation, the procedure (or algorithm) described in the last section is the most complex, but the most important one. However, each of the four methods builds on the previous one. A code developer may thus choose to implement all the four cases below as a testing method for the general case.

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## 1 Well-posedness for transmission problems in isotropic weighted Sobolev spaces

While we are interested in this paper mostly in the mesh refinement, we include first some regularity results for transmission problems, since transmission problems have not been studied as much as their practical importance would warrant it. The remaining sections will deal exclusively with mesh refinement. See [1] for a more theoretical review of these problems.

We shall use the standard notation for partial derivatives, i.e.,  $\partial_j = \frac{\partial}{\partial x_j}$  and  $\partial^\alpha = \partial_1^{\alpha_1} \dots \partial_d^{\alpha_d}$ . For a multi-index  $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{Z}_+^d$ , we denote the usual Sobolev spaces on an open set  $\Omega \subset \mathbb{R}^d$  by

$$H^m(\Omega) = \{u : \Omega \rightarrow \mathbb{C}, \partial^\alpha u \in L^2(\Omega), |\alpha| \leq m\}.$$

The solution of an elliptic equation can be singular in various practical situations. Some typical examples are: singularities due to the non-smoothness of domain with Dirichlet boundary conditions, singularities due to the change of boundary conditions, singularities due to non-smooth corners with adjacent Neumann conditions, and singularities due to the non-smoothness of the interface in transmission problems. To improve the regularity of problem (1) in the presence of this type of singularities, we consider *weighted Sobolev spaces*. First, we need to introduce more formally the notion of *singular boundary points* of the domain  $\Omega \subset \mathbb{R}^d$ .

### 1.1 Weighted Sobolev spaces

We introduce  $\partial_{\text{sing}}\Omega \subset \partial\Omega$  to be the set of non-smooth (or singular) boundary points of  $\Omega$ . More precisely,  $\partial_{\text{sing}}\Omega$  is the union of the set of vertices and of other singular points (for instance where the boundary conditions change or where an interface or crack touch the boundary). In three dimensions, the set  $\partial_{\text{sing}}\Omega$  will be the union of the edges and the set where the boundary conditions change and of other singular points. More precisely, the set  $\mathcal{V}$  of all singular points will also include the nonsmooth points of the interfaces, of the cracks, or of the potential  $V$  (if  $V \neq 0$ ).

Let us denote by  $r_\Omega(x)$  the distance from a point  $x \in \Omega$  to the set  $\mathcal{V}$ . We agree to take  $r_\Omega = 1$  if  $\mathcal{V}$  is empty, that is, if  $\partial\Omega$ , the interface, and  $V$  are smooth, the interface does not touch the boundary, and there are no cracks. Then, for  $\mu \in \mathbb{Z}_+$  and  $a \in \mathbb{R}$ , we define the weighted Sobolev space  $\mathcal{K}_a^\mu(\Omega)$  by

$$\mathcal{K}_a^\mu(\Omega) := \{u \in L_{\text{loc}}^2(\Omega), r_\Omega^{|\alpha|-a} \partial^\alpha u \in L^2(\Omega), \text{ for all } |\alpha| \leq \mu\}. \quad (3)$$

These spaces are also called *Babuška-Kondratiev* spaces. The space  $\mathcal{K}_a^\mu(\Omega)$  is endowed with the induced Hilbert space norm. For  $s \in \mathbb{R}_+$ , the space  $\mathcal{K}_a^s(\partial\Omega)$  are defined by standard (real method of) interpolation. For  $s < 0$  these spaces are defined by duality (as usual).

## 1.2 Transmission problems

Let us assume that  $\Omega$  is the union of some polygonal domains  $\Omega_j$  with disjoint interiors. Let us assume that  $A$  is a constant on each subdomain and that  $V$  has only jump discontinuities at the interface separating the domains  $\Omega_j$ . Then we consider the problem

$$Lu := -\nabla(A\nabla u) + Vu = f \text{ in } \Omega \quad (4)$$

with mixed boundary conditions. We shall also need the *broken Sobolev* spaces

$$\hat{\mathcal{K}}_a^m(\Omega) := \{u \in \mathcal{K}_a^m(\Omega_j), \text{ for all } j\}. \quad (5)$$

## 1.3 Adjacent Neumann faces and non-smooth interfaces in 2D

To obtain a well-posedness result for interface problems in 2D, we can proceed as follows [12]. For any non-smooth point  $P$ , let  $\chi_P$  be a smooth function that is equal to 1 near  $P$ . We assume that the function  $\chi_P$  have disjoint supports. Let  $W_s$  be the linear span of the functions  $\chi_P$  corresponding to a singular point  $P$  that is either a point where we have adjacent Neumann-Neumann conditions or a non-smooth interface point satisfying respectively Neumann boundary conditions on the sides at  $P$ . This includes points  $P$  that belong to more than two of the subdomains  $\bar{\Omega}_j$  (so called *multiple junction points*). Thus for the pure Dirichlet problem (and no interfaces)  $W_s = 0$ , whereas for the pure Neumann problem, the dimension of  $W_s$  is the same as that of the number of singular points. Let  $L$  and  $A$  be as in Equation (4) and

$$\mathcal{D}_a := \{u \in \hat{\mathcal{K}}_{a+1}^{m+1}(\Omega) \cap \mathcal{K}_{a+1}^1(\Omega), u^+ = u^-, A^+ \partial_\nu u = A^- \partial_\nu u \text{ on } \Gamma\}. \quad (6)$$

The following result is new. It can be proved by combining the techniques of [12] and [13].

Let  $\partial_D \Omega$  and  $\partial_N \Omega := \partial\Omega \setminus \partial_D \Omega$  be the Dirichlet part of the boundary (assumed to be closed without isolated points and a union of segments). Let us denote by  $\tilde{L}u = (Lu, u|_{\partial_D \Omega}, \partial_\nu \Omega|_{\partial_N \Omega})$ , where  $\partial_\nu$  is the normal derivative at the boundary.

**Theorem 1.1.** *Let  $\Omega$  be a domain with a polygonal structure. Then, there exists  $\eta > 0$  such that, for all any  $0 < a < \eta$  and  $m \in \mathbb{Z}_+$ , the map*

$$\tilde{L} : \mathcal{D}_a + W_s \rightarrow \hat{\mathcal{K}}_{a-1}^{m-1}(\Omega) \oplus \mathcal{K}_{a+1/2}^{m+1/2}(\partial_D \Omega) \oplus \mathcal{K}_{a-1/2}^{m-1/2}(\partial_N \Omega),$$

with  $\mathcal{D}_a$  given in (6), is an isomorphism.

The importance of combining transmission problems with singular potentials is that, if one considers the Neumann problem and wants to replace it with an equation that gives a one-to-one map, then necessarily  $V$  will have singularities of the form  $1/r^2$  at all the points of  $\mathcal{V}$ . This procedure is similar with the one that replaces the Neumann Laplacian  $-\Delta$  with  $1 - \Delta$  to achieve an operator with a unique solution.

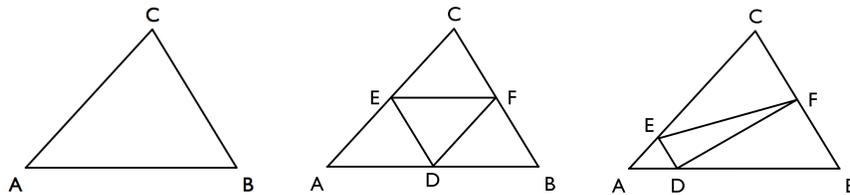


Figure 2.1: The initial triangle  $ABC$  (left); the uniform refinement,  $\kappa = 0.5$  (center); the  $\kappa$ -refinement with  $\kappa < 0.5$  for vertex  $A$  (right),  $\kappa = \frac{|AD|}{|AB|} = \frac{|AE|}{|AC|} = \frac{|DE|}{|BC|}$ .

## 2 Optimal 2D graded meshes

Theorem 1.1 can be used to justify the construction of a sequence of meshes in 2D that yields  $h^m$ -quasi-optimal rates of convergence for transmission problems with non-smooth interfaces (and even with multiple junctions). We notice that the resulting sequence of meshes is the same for all 2D problems on polygonal domains, although the theoretical *a priori* estimates are different for the pure Dirichlet and the pure Neumann problems. The same constructions will apply to Schrödinger operators with inverse square potentials in two dimensions. We thus now present a systematic construction of graded meshes that yield quasi-optimal rates of convergence in 2D for problems that combine both jump discontinuities in the diffusion coefficient and singular potentials.

Recall from Section 1 the set of singular points  $\mathcal{V} \supset \partial_{\text{sing}}\Omega$  associated to our problem. For Schrödinger operators, we include the singular points of the potential  $V$  in the set  $\mathcal{V}$ .

**Definition 2.1.** Let  $\kappa \in (0, 1/2]$  for each  $Q \in \partial_{\text{sing}}\Omega$ , and  $\mathcal{T}$  be a triangulation of  $\Omega$ . We require that every singular point in  $\mathcal{V}$  be a vertex in  $\mathcal{T}$  and no two singular points belong to the same triangle. Then the  $\kappa$ -refinement of  $\mathcal{T}$ , denoted by  $\kappa(\mathcal{T})$  is obtained by dividing each edge  $AB$  of  $\mathcal{T}$  in two parts as follows. If neither  $A$  nor  $B$  is a singular point, then we divide  $AB$  into two equal parts. Otherwise, if say  $A \in \mathcal{V}$  (so  $A$  is a singular point), we divide  $AB$  into  $AC$  and  $CB$  such that  $|AC| = \kappa|AB|$ . This procedure will divide each triangle of  $\mathcal{T}$  into four triangles.

The mesh refinement described in Definition 2.1 is illustrated in Figure 2.1.

*Remark 2.2.* To achieve the optimal convergence rate in the finite element method, near a singular point, we can choose  $\kappa = \min(1/2, 2^{-m/a})$ , for any  $0 < a < \min(m, \eta)$ , where  $m$  is the degree of polynomials used in the finite element method. Although it seems that any positive  $a < \min(m, \eta)$  can be taken to calculate  $\kappa$ , the smaller the value of  $a$ , the less shape-regularity we will have in triangulation. Since regularity is a local property, we may allow different grading parameters  $\kappa_i$  near different singular points. In this case,  $\kappa_i$  is determined similarly by some local regularity indices near each singular point. See [12] for detailed discussions on these local indices.

Now, we define the graded mesh based on successive  $\kappa$ -refinements.

**Definition 2.3.** For a fixed  $m = \{1, 2, \dots\}$ , we define a sequence of meshes  $\mathcal{T}_n$  as follows. The initial mesh  $\mathcal{T}_0$  is such that every singular point in  $\mathcal{V}$  has to be the vertex of a triangle in the mesh and all interfaces coincide with edges in the mesh. In addition, we chose  $\mathcal{T}_0$  such that there is no triangle that contains more than one singular point. Then, we define by induction  $\mathcal{T}_{n+1} = \kappa(\mathcal{T}_n)$ .

The following theorem ensures the optimality of the finite element approximation to singular solutions of transmission problems on these graded meshes.

**Theorem 2.4.** *Let  $m$  be the degree of polynomials in finite element method and let  $u_n$  be the finite element solution of the transmission problem (4) on the graded mesh  $\mathcal{T}_n$  defined above. Then, assuming the zero Dirichlet boundary condition,*

$$\|u - u_n\|_{H^1(\Omega)} \leq C \dim(S_n)^{-m/2} \|f\|_{H^{m-1}(\Omega)},$$

where  $S_n$  is the finite element space associated with the triangulation,  $f$  is the given data in the PDE, and  $C$  is a constant independent of  $f$  and  $n$ .

See [12] and [13] for numerical tests verifying the results of the above theorem in particular cases.

### 3 Schrödinger operators with inverse square potentials in 3D

We now consider the case of Schrödinger operators in three dimensions with periodic boundary conditions. We define our Sobolev spaces similarly, but using periodic functions and integration on the fundamental domain. In this case  $\mathcal{V} = \mathcal{S}$ , the set of singular points of the potential  $V$ .

#### 3.1 Schrödinger operators

Consider the Hamiltonian operator  $H := -\Delta + V$  that is periodic on  $\mathbb{R}^3$  with periodicity lattice  $\Lambda$ . Its fundamental domain is a parallelepiped whose faces can be identified under the symmetries of  $H$  to form the torus  $\mathbb{T} = \mathbb{R}^3/\Lambda$ , which is how we will denote this fundamental domain throughout the paper. Let  $\mathcal{S} \subset \mathbb{T}$  be a discrete set of finite points. Let  $\rho(x)$  be a continuous function on  $\mathbb{T}$  that is given by  $\rho(x) = |x - p|$  for  $x$  close to  $p \in \mathcal{S}$ , which is smooth except at the points in  $\mathcal{S}$ , and may be assumed to be equal to one outside a neighborhood of  $\mathcal{S}$ . We assume that the periodic potential  $V$  has the following property:  $\rho^2 V$  is continuous across  $p \in \mathcal{S}$  and smooth in polar coordinates around  $p$ . The weighted Sobolev spaces are defined as in Equation (3), but using the function  $\rho$  instead of  $r_\Omega$ .

These Hamiltonian operators with inverse square potentials arise in a variety of interesting contexts. The standard example of a Schrödinger operator with  $c/\rho$  potential is a special case of the inverse square potentials we consider, where the function  $\rho^2 V$  vanishes to order 1 at the singularity. But in addition, Hamiltonians with true inverse square potentials arise in relativistic quantum mechanics from the square of the Dirac operator coupled with an interaction potential, and they arise in the interaction of a polar molecule with an electron.

In some practical problems the function  $\rho^2 V$  may be negative at some points  $p \in \mathcal{S}$ . We present next a careful examination on the well-posedness of the equation  $Hu = f$  that includes also the possibility that  $\rho^2 V$  takes negative values at some singular points. The following result holds with mild restrictions on the potential  $V$  [7].

**Theorem 3.1.** *Suppose  $\eta_0 := \min_{p \in \mathcal{S}} \rho^2 V(p) > -1/4$ . Let  $\eta := \sqrt{1/4 + \eta_0}$ . Then there exists  $C_0 > 0$  such that  $L + H : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S}) \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus \mathcal{S})$  is an isomorphism for all  $m \in \mathbb{Z}_{\geq 0}$ , all  $|a| < \eta$ , as long as  $L > C_0$ .*

In addition to the well-posedness of the 3D Schrödinger equation with inverse square potentials, this theorem shall justify the construction of 3D graded tetrahedra in the finite element approximation both to the solution and to the eigenvalue problem associated to the operator.

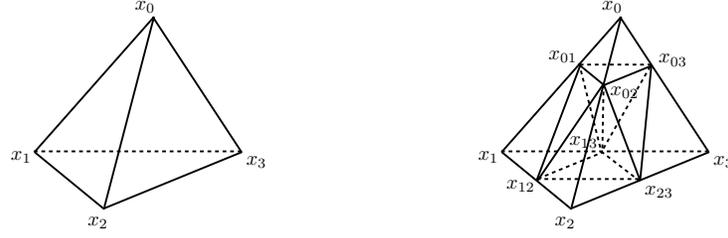


Figure 3.1: The initial tetrahedron  $\{x_0, x_1, x_2, x_3\}$  (left); eight sub-tetrahedra after one  $\kappa$ -refinement (right),  $\kappa = \frac{|x_0 x_{01}|}{|x_0 x_1|} = \frac{|x_0 x_{02}|}{|x_0 x_2|} = \frac{|x_0 x_{03}|}{|x_0 x_3|}$ .

### 3.2 Graded tetrahedral meshes

In view of Theorem 3.1, the solution  $u$  of the Schrödinger equation is defined in the weighed space and therefore it may not be sufficiently smooth. This actually decreases the efficiency of the finite element approximation. We here develop the 3D analogy of the 2D graded mesh in Definition 2.3, such that the optimal convergence rate can be obtained in the associated finite element approximation.

We keep the degree  $m$  of polynomials in the approximation fixed. Choose  $a$  such that  $0 < a < \eta := \min_{p \in \mathcal{S}} \sqrt{1/4 + \rho^2 V(p)}$  and  $a \leq m$  and let  $k = 2^{-m/a}$ . Denote by  $\mathbb{P}$  a parallelepiped that is a fundamental domain of the Lattice  $\Lambda$ . Choose an initial mesh  $\mathcal{T}_0$  of  $\mathbb{P}$  with tetrahedra such that all singular points of  $V$  (i.e., all points of  $\mathcal{S}$ ) are among the vertices of  $\mathcal{T}_0$  and no tetrahedron has more than one vertex in  $\mathcal{S}$ . We assume that this mesh is such that if  $F_1$  and  $F_2$  are two opposite faces of  $\mathbb{P}$ , which hence correspond to each other through periodicity, then the resulting triangulations of  $F_1$  and  $F_2$  will also correspond to each other, that is, they are congruent in an obvious sense.

We start with a special refinement of an arbitrary tetrahedron  $T$  that has one of the vertices in the set  $\mathcal{S}$ . Our assumptions then guarantee that all the other vertices of  $T$  will not be in  $\mathcal{S}$ . Then, we define our  $\kappa$ -refinement algorithm for a single tetrahedron that divides  $T$  into eight sub-tetrahedra as follows.

**Algorithm 3.2.  $\kappa$ -refinement for a single tetrahedron:** Let  $x_0, x_1, x_2, x_3$  be the four vertices of  $T$ . We denote  $T$  by its vertex set  $\{x_0, x_1, x_2, x_3\}$ . Suppose that  $x_0 \in \mathcal{S}$ , so that  $x_0$  is the one and only vertex that will be refined with a ratio  $\kappa \in (0, 1/2]$ . We first generate new nodes  $x_{ij}$ ,  $0 \leq i < j \leq 3$ , on each edge of  $T$ , such that  $x_{ij} = (x_i + x_j)/2$  for  $1 \leq i < j \leq 3$  and  $x_{0j} = (1 - \kappa)x_0 + \kappa x_j$  for  $1 \leq j \leq 3$ . Note that the node  $x_{ij}$  is on the edge connecting  $x_i$  and  $x_j$ . Connecting these nodes  $x_{ij}$  on all the faces, we obtain 4 sub-tetrahedra and one octahedron. The octahedron then is cut into four tetrahedra using  $x_{13}$  as the common vertex. Therefore, after one refinement, we obtain eight sub-tetrahedra (Figure 3.1), namely,

$$\begin{aligned} & \{x_0, x_{01}, x_{02}, x_{03}\}, \{x_1, x_{01}, x_{12}, x_{13}\}, \{x_2, x_{02}, x_{12}, x_{23}\}, \{x_3, x_{03}, x_{13}, x_{23}\} \\ & \{x_{01}, x_{02}, x_{03}, x_{13}\}, \{x_{01}, x_{02}, x_{12}, x_{13}\}, \{x_{02}, x_{03}, x_{13}, x_{23}\}, \{x_{02}, x_{12}, x_{13}, x_{23}\}. \end{aligned}$$

**Algorithm 3.3.  $\kappa$ -refinement for a mesh:** Let  $\mathcal{T}$  be a triangulation of the domain  $\mathbb{P}$  such that all points in  $\mathcal{S}$  are among the vertices of  $\mathcal{T}$  and no tetrahedron contains more than one point in  $\mathcal{S}$  among its vertices. Then we divide each tetrahedron  $T$  of  $\mathcal{T}$  that has a vertex in  $\mathcal{S}$  using the  $\kappa$ -refinement and we divide each tetrahedron in  $T$  that has no vertices in  $\mathcal{S}$  using the  $1/2$ -refinement. The resulting mesh will be denoted by  $\kappa(\mathcal{T})$ . We then define  $\mathcal{T}_n = \kappa^n(\mathcal{T}_0)$ , where  $\mathcal{T}_0$  is the initial mesh of  $\mathbb{P}$ .

*Remark 3.4.* According to [3], when  $\kappa = 1/2$ , which is the case when the tetrahedron under consideration is away from  $\mathcal{S}$ , the recursive application of Algorithm 3.2 on the tetrahedron generates tetrahedra within at most three similarity classes. On the other hand, if  $\kappa < 1/2$ , the eight sub-tetrahedra of  $T$  are not necessarily similar. Thus, with one  $\kappa$ -refinement, the sub-tetrahedra of  $T$  may belong to at most eight similarity classes. Note that the first sub-tetrahedra in Algorithm 3.2 is similar to the original tetrahedron  $T$  with the vertex  $x_0 \in \mathcal{S}$  and therefore, a further  $\kappa$ -refinement on this sub-tetrahedron will generate eight children tetrahedra within the same eight similarity classes as sub-tetrahedra of  $T$ . Hence, successive  $\kappa$ -refinements of a tetrahedron  $T$  in the initial triangulation  $\mathcal{T}_0$  will generate tetrahedra within at most three similarity classes if  $T$  has no vertex in  $\mathcal{S}$ . On the other hand, successive  $\kappa$ -refinements of a tetrahedron  $T$  in the initial triangulation will generate tetrahedra within at most  $1 + 7 \times 3 = 22$  similarity classes if  $T$  has a point in  $\mathcal{S}$  as a vertex. Thus, our  $\kappa$ -refinement is conforming and yields only non-degenerate tetrahedra, all of which will belong to only finitely many similarity classes.

*Remark 3.5.* Recall that our initial mesh  $\mathcal{T}_0$  has matching restrictions to corresponding faces. Since the singular points in  $\mathcal{S}$  are not on the boundary of  $\mathbb{P}$ , the refinement on opposite boundary faces of  $\mathbb{P}$  is obtained by the usual mid-point decomposition. Therefore, the same matching property will be inherited by  $\mathcal{T}_n$ . In particular, we can extend  $\mathcal{T}_n$  to a mesh in the whole space by periodicity. We will, however, not make use of this periodic mesh on the whole space.

Then, the optimal convergence rate is obtained by the finite element approximation of the Schrödinger equation on our 3D graded meshes.

**Theorem 3.6.** *The sequence  $\mathcal{T}_n := \kappa^n(\mathcal{T}_0)$  of meshes on  $\mathbb{P}$  defined using the  $\kappa$ -refinement, for  $\kappa = 2^{-m/a}$ ,  $0 < a < \eta$ ,  $a \leq m$ , has the following property. Using piecewise polynomials of degree  $m$ , the sequence  $u_n \in S_n$  of finite element (Galerkin) approximations of  $u$  from the equation  $(L + H)u = f$  satisfies*

$$\|u - u_n\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} \leq C \dim(S_n)^{-m/3} \|f\|_{\mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus \mathcal{S})}, \quad (7)$$

where  $S_n$  is the finite element space associated with  $\mathcal{T}_n$  and  $C$  is independent of  $n$  and  $f$ .

One of the consequences of Theorem 3.6 is that the eigenpairs of the Schrödinger operator can also be approximated using the finite element method on graded tetrahedra in the optimal rate [8].

#### 4 Quasi-optimal $h^m$ -mesh refinement on 3D polyhedra

We describe now an algorithm to obtain quasi-optimal  $h^m$ -mesh refinement. We extend the procedure in Section 3, following [2], from where the pictures are taken. The theoretical justification for this algorithm is based on the anisotropic regularity result of [2], where the anisotropic weighted Sobolev spaces  $\mathcal{D}_a^m(\Omega)$  were introduced. More precisely, given a bounded polyhedral domain  $\Omega$  and a parameter  $\kappa \in (0, 1/2]$ , we will provide a sequence  $\mathcal{T}_n$  of meshes of  $\Omega$  composed of finitely many tetrahedra, such that, if  $S_n$  is the finite element space of continuous, piecewise polynomials of degree  $m$  on  $\mathcal{T}_n$ , then the Lagrange interpolant of  $u$  of order  $m$ ,  $u_{I,n}$ , has  $h^m$ -quasi-optimal approximability properties.

**Theorem 4.1.** *Let  $\kappa \in (0, 1/2]$  and  $0 < \kappa \leq 2^{-m/a}$ . Then there exists a sequence of meshes  $\mathcal{T}_n$  and a constant  $C > 0$  such that, for the corresponding sequence of finite element spaces  $S_n$ , we have*

$$|u - u_{I,n}|_{H^1(\Omega)} \leq C 2^{-nm} \|u\|_{\mathcal{D}_{a+1}^{m+1}(\Omega)},$$

for any  $u \in \mathcal{D}_{a+1}^{m+1}(\Omega)$ ,  $u|_{\partial\Omega} = 0$ , and for any  $m \in \mathbb{Z}_+$ . Moreover,  $\dim(S_n) \sim 2^{3n}$ , where  $S_n$  are the associated finite element spaces.

The desired relation (2) is now a direct consequence of Theorem 4.1 and of Céa's Lemma.

#### 4.1 Refinement Strategy

Following [2], we describe now our refinement strategy. The refinement strategy will inductively generate a sequence of decompositions  $\mathcal{T}'_n$  of  $\Omega$  in tetrahedra and triangular prisms, while our meshes  $\mathcal{T}_n$  will be obtained by further dividing each prism in  $\mathcal{T}'_n$  into three tetrahedra. We now explain how the divisions  $\mathcal{T}'_n$  are defined,  $\mathcal{T}'_{n+1}$  being a refinement of  $\mathcal{T}'_n$  in which each edge is divided into two (possibly unequal) edges as in the 2D case.

More precisely, to define the way each edge of  $\mathcal{T}'_n$  is divided, we need to establish a hierarchy of the nodes of  $\mathcal{T}'_n$ , some nodes being “more singular” than the others. We proceed as follows. Given a point  $P \in \bar{\Omega}$ , we shall say that  $P$  is of *type V* if it is a vertex of  $\Omega$ ; we shall say that  $P$  is of *type E* if it is on an open edge of  $\Omega$ . Otherwise, we shall say that it is of *type S* (that is, a “smooth” point). The type of a point depends only on  $\Omega$  and our problem, Equation (1), and will not depend on any partition or meshing.

We denote each edge in the mesh by its endpoints. Then, the initial tetrahedralization will consist of edges of type **VE**, **VS**, **ES**, **EE**:=**E**<sup>2</sup>, and **S**<sup>2</sup>. We assume that our initial decomposition and initial tetrahedralization were defined so that no edges of type **V**<sup>2</sup> := **VV** are present. The points of type **V** will be regarded as more singular than the points of type **E**, and the points of type **E** will be regarded as more singular than the points of type **S**. Namely, **V** > **E** > **S**. All the resulting triangles in our mesh will hence be of one of the types **VES**, **VSS**, **ESS**, and **SSS**. We can assume that there are no triangles of type **EES**.

As in the other refinements considered in our paper, our refinement procedure depends on the choice of a constant  $\kappa \in (0, 2^{-m/a})$ , where  $a > 0$  is as in the anisotropic regularity estimate of  $u$  [2] and  $\kappa \leq 1/2$  ( $a$  is as in Theorem 4.1). We can improve our construction by considering different values of  $\kappa$  associated to different vertices or edges. See [12] for example. Let  $AB$  be a generic edge in the decompositions  $\mathcal{T}_n$ . Then, as part of the  $\mathcal{T}_{n+1}$ , this edge will be decomposed in two segments as follows. If  $A$  is more singular than  $B$  (i.e., if  $AB$  is of type **VE**, **VS**, or **ES**),  $AB$  is divided into  $AC$  and  $CB$ , such that  $|AC| = \kappa|AB|$ . Except when  $\kappa = 1/2$ ,  $C$  will be closer to the more singular point. This procedure is similar to the 2D procedure considered in Section 2. See Figure 4.1.

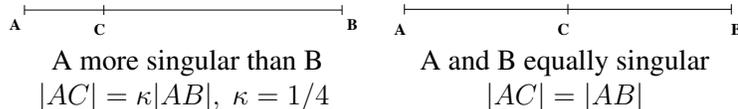
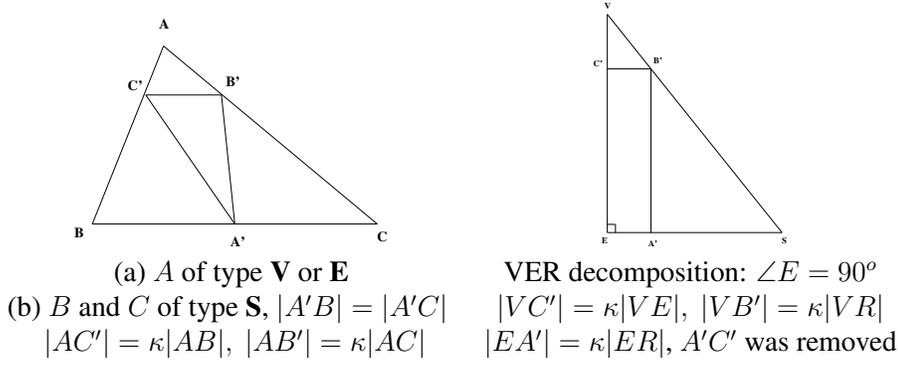


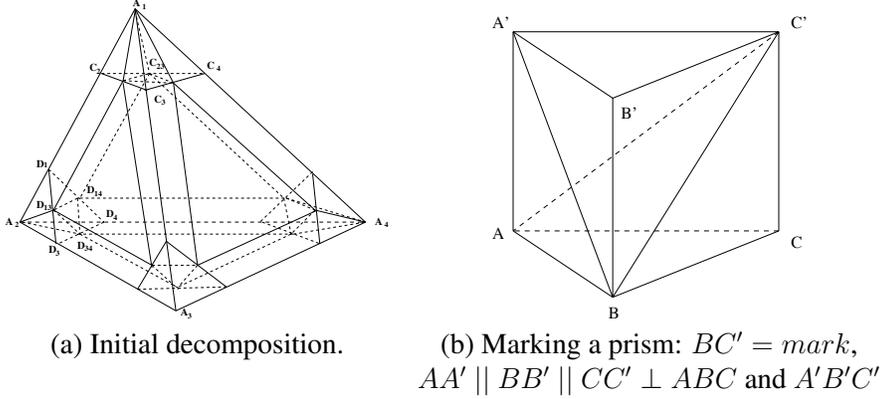
Figure 4.1: Edge decomposition

The above strategy to refine the edges induces a natural strategy for refining the triangular faces. If  $ABC$  is a triangle in the decomposition  $\mathcal{T}'_n$ , then in  $\mathcal{T}'_{n+1}$ , the triangle  $ABC$  will be divided into four smaller triangles, according to the vertex type. The decomposition of triangles of type **S**<sup>3</sup> is obtained for  $\kappa = 1/2$ . The type **VSS** triangle decomposition is described in Figure 4.2 (a). In the case when  $ABC$  is of type **VES**, however, we use a different construction as follows. We remove the newly introduced segment that is opposite to  $B$ , see Figure 4.2 (b), and divide  $ABC$  into two triangles and a quadrilateral. The resulting quadrilateral will belong to a prism in  $\mathcal{T}'_{n+1}$ .


 Figure 4.2: Triangle decomposition,  $\kappa = 1/4$ 

## 4.2 Divisions in tetrahedra and prisms

We now describe the construction of the sequence of the decompositions  $\mathcal{T}'_n$  for  $n \geq 0$ . The required mesh refinement will be obtained by dividing all the prisms in  $\mathcal{T}'_n$  into tetrahedra.

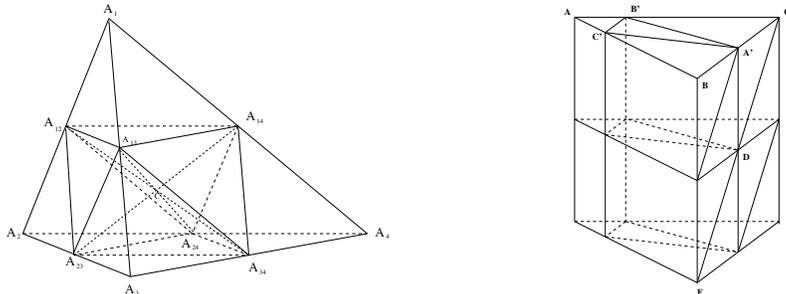

 Figure 4.3: The initial decomposition  $\mathcal{T}'_0$  of  $\Omega$ .

We start with an initial division  $\mathcal{T}'_0$  of  $\Omega$  in straight triangular prisms and tetrahedra of types **VESS** and **VS<sup>3</sup>**, having a vertex in common with  $\Omega$ , and an interior region  $\Lambda_0$ . See Figure 4.2 (a), where we have assumed that our domain  $\Omega$  is a tetrahedron. For each of the prisms we choose a diagonal (called mark) which will be used to uniquely define a partition of the triangular prism into tetrahedra. We then divide the interior region  $\Lambda_0$  into tetrahedra that will match the marks. Also, we assume that the marks on adjacent prisms are compatible, so that the resulting meshes are conforming. We can further assume that some of the edge points (as in Figure 4.2 (b)) have been moved along the edges so that the prisms become straight triangular prisms *i.e.*, the edges are perpendicular to the bases.

The decompositions  $\mathcal{T}'_n$  are then obtained by induction following the steps below. We assume that the decomposition  $\mathcal{T}'_n$  was defined and we proceed to define the decomposition  $\mathcal{T}'_{n+1}$ .

**Step 1.** A tetrahedron of type **S<sup>4</sup>** is refined uniformly by dividing along the planes given by  $t_i + t_j = k/2^n$ ,  $1 \leq k \leq 2^n$ ,  $k \in \mathbb{Z}$ , where  $[t_0, t_1, t_2, t_3]$  are affine barycentric coordinates. See Figure 4.2 (a) for  $n = 1$ . This is similar to the procedure used in Section 3 and is compatible with the already defined refinement procedure for the faces.

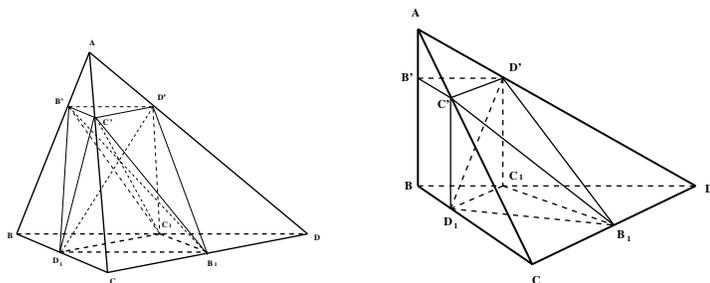
**Step 2.** We perform semi-uniform refinement for prisms in our decomposition  $\mathcal{T}'_n$  (all these prisms will have an edge in common with  $\Omega$ ). This procedure is shown in Figure 4.2 (b) and is again compatible with the already defined refinement procedure for the faces.



(a) First level of uniform refinement (b) First level of semi-uniform refinement of a prism,  $CD = mark$

Figure 4.4: First refinement  $\mathcal{T}'_1$ .

**Step 3.** We perform non-uniform refinement for the tetrahedra of type  $\mathbf{VS}^3$  and  $\mathbf{VESS}$ . More precisely, we divide a tetrahedron of type  $\mathbf{VS}^3$  into 12 tetrahedra as in the uniform strategy, but with the edges through the vertex of type  $\mathbf{V}$  divided in the ratio  $\kappa$ . We thus obtain one tetrahedron of type  $\mathbf{VS}^3$  as in Section 3. We then obtain 11 tetrahedra of type  $\mathbf{S}^4$ . See Figure 4.2 (a). On the other hand, a tetrahedron of type  $\mathbf{VESS}$  will be divided into 6 tetrahedra of type  $\mathbf{S}^4$ , one tetrahedron of type  $\mathbf{VS}^3$ , and a triangular prism. The vertex of type  $\mathbf{E}$  will belong only to the prism. See Figure 4.2 (b). This refinement is compatible with the earlier refinement of the faces.



(a) Vertex A of type  $\mathbf{V}$ , B, C, D of type  $\mathbf{S}$  (b) Vertex A of type  $\mathbf{V}$ , B of type  $\mathbf{E}$ , C, D of type  $\mathbf{S}$  and  $D_1D' = mark$  for the prism  $BD_1C_1D'C_1B'$

Figure 4.5: Refinement of tetrahedra of type  $\mathbf{VS}^3$  and  $\mathbf{VESS}$ .

The description of our refinement procedure is now complete.

### 4.3 Intrinsic local refinement

One of the main features of our refinement is that each edge, each triangle, and each quadrilateral that appears in a tetrahedron or prism in the decomposition  $\mathcal{T}'_n$  is divided in the decomposition  $\mathcal{T}'_{n+1}$  in an intrinsic way that depends only on the type of the vertices of that edge, triangle, or quadrilateral. In particular, the way that a face in  $\mathcal{T}'_n$  is divided to yield  $\mathcal{T}'_{n+1}$  does

not depend on the type of the other vertices of the tetrahedron or prism to which it belongs. This ensures that tetrahedralization  $\mathcal{T}_{n+1}$ , which is obtained from  $\mathcal{T}'_{n+1}$  by dividing each prism in three tetrahedra, is a conforming mesh.

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