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Self-adjointness and spectrum of Stark operators on finite intervals

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Abstract

In this paper, we study self-adjointness and spectrum of operators of the form

$$H = -\frac{d^2}{dx^2} + Fx, F > 0 \quad \text{on} \quad \mathcal{H} = L^2(-L, L).$$

H is called Stark operator and describes a quantum particle in a quantum asymmetric well. Most of known results on mathematical physics does not take in consideration the self-adjointness and the operating domains of such operators. We focus on this point and give the parametrization of all self-adjoint extensions. This relates on self-adjoint domains of singular symmetric differential operators. For some of these extensions, we numerically, give the spectral properties of H. One of these examples performs the interesting phenomenon of splitting of degenerate eigenvalues. This is done using the a combination of the Bisection and Newton methods with a numerical accuracy less than 10^{-8}.

Keywords Spectral theory, Shrödinger operators, Stark operators, self-adjointness, Symmetric differential operators, Airy functions
AMS Subject Classifications 34B24, 47E05

1 Introduction

The study of self-adjoint domains of symmetric differential operators on Hilbert spaces is a central problem in the theory of partial differential operators. It has a deep background in mathematical physics. As it is already mentioned in [26], a lot of works confuse between the symmetry (Hermiticity) and the self-adjointness, which leads to a non precise and even incomplete results. Frequently the basic distinction between unbounded and bounded operators is not considered, or often it is neglected. For getting a self-adjoint operator, the

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symmetric condition for unbounded operator is in general not sufficient. For differential operators on bounded domains the boundaries conditions at the end of the interval can change the situation and the question of self-adjointness it becomes more subtle and there are several scenarios, and the presence of boundaries changes significantly the picture. The operator can be self-adjoint, essentially self-adjoint, having many self-adjoint extensions or no self-adjoint extension at all or even non symmetric. So in this situation, we need more analysis to characterize a truly self-adjoint operator. In fact, if an observable of a quantum system is constructed starting from a symmetric operator will not be able to give the result performing measurement of such observable until we have made precise which self-adjoint extension of the system operator represents the observable.

One could ask, why the self-adjoint property is important? To convince the readers of the importance of this subject, we perform two fundamental reasons:

- It is well-known that in mathematical physics problems we are interested in, are observable with real spectrum, which are guaranteed only for self adjoint operators. Thus it is very important to know if the domains under which theses operators are self-adjoint. Outside theses domains, eigenvalues are not only real-valued, and hence the operators cannot be considered as physical operators.
- Every self-adjoint operator is the generator of a unitary group. Indeed when H is a self-adjoint operator, the operators

$$U_t = \exp(itH), \quad t \in \mathbb{R};$$

are a (strongly continuous one-parameter) unitary group, and H is its generator [27]. More generally an operator generates a unitary group if and only if it is self-adjoint. This is could be related to the existence of dynamics in quantum mechanics. Not only the dynamical evolution is affected by the determination of the boundary conditions, or the self-adjoint extensions of families of symmetric operators, but also the results of the measures realized on the system and also the measurable quantities of the system [16].

1.1 Stark operators on finite intervals

Experimentally, the atomic Stark effect means the shifts viewed in atomic emission spectra after placing the particle in a constant electric field of strength F. J. Stark, in the non-relativistic quantum theory, this Stark effect is usually modeled by an Hamiltonian operator that (in appropriately scaled units and with the atomic units $2m = h = q = 1$ to simplify the equation) has the form

$$H(F) = -\Delta + V(x) + Fx. \tag{1}$$

Hamiltonian that is parameterized by operators of the form (1) has been intensively studied in the last five decinies [18, 23] and references therein. A quantum well is a particular kind of structure in which one layer is surrounded by two barrier layers. Theses layers, in which particles are confined, could be so thin that we cannot neglect the fact that particles are waves. In fact, the allowed states in this structure correspond to standing waves in the direction perpendicular to the layers. Mathematically this corresponds to the study of (1) on a $L^2(I)$, with I is a finite interval seen as the support of V (known as the quantum well). Basic properties of a quantum well could be studied through the simple particle in a box model. In the case of infinite quantum well it is expected that the energy levels are quadratically spaced, the energy level spacing becomes large for narrow wells.

When electric field is applied to quantum wells, their optical absorption spectrum near to the band-gap energy can be changed considerably [18, 23], an effect known as electro-absorption.

The correct results in that case can also be obtained by explicit expansion of the exact eigenvalue condition, but this requires knowing the properties of the boundary behavior and self-adjointness and the domain of the operator. This is the subject of the present paper. In the following section we summarize related results and give a brief survey of literature.

1.2 Self-adjointness

The analysis of self-adjointness and the role of the boundary in quantum systems has became a recent focus of activity in different branches [3] and references therein. Everitt in [10] gave some results on self-adjoint domains under the assumption of the limit circle case and the limit point case. Using the Glazman-Krein-Naimark theory Everitt et al. in [11] showed that there exists a one-to-one correspondence between the set of all the self-adjoint extensions of a minimal operator generated by quasi-differential expressions and the set of all the complete Lagrangian subspaces of a related boundary space. They used symplectic geometry. Sun et al [31, 35, 36] presented a complete and cordial characterization of all self-adjoint extensions of symmetric differential operators. This is done by giving a new decomposition of the maximal operator domain. The later result is generalized by Evans and Ibrahim in [9]. Fu in [14] gives the characterizations of self-adjoint domains for singular symmetric operators by describing boundary conditions of domain of conjugate differential operator, with singular points. Most of These operators are defined on a weighted Hilbert function space. Self-adjointness of momentum operators in generalized coordinates is given in [7] and of curl operator in [15].
In [4], the authors consider a Schrödinger operator with a magnetic field and no electric field on a domain in the Euclidean space with compact boundary. They give sufficient conditions on the behavior of the magnetic field near the boundary which guarantees essential self-adjointness of the operator. The problem concerning scalar potentials is first studied in [25, 29], under sum assumption on the behavior of V when approaching the boundary. In [8], a characterization was given for symmetric even order elliptic operators in bounded regular domains. Recently in [12], the authors established a bijection between the self-adjoint of the Laplace operator on bounded regular domain and the unitary operator on the boundary. In [17], Katsnelson consider the formal prolate spheroid differential operator on a finite symmetric interval and describes the self-adjoint boundary conditions. He proves that among all self-adjoint extensions there is a unique realization which lead to an operator commuting with the Fourier operator trounced on the considered interval. In [5], a self-adjoint extensions is considered for analyzing momentum and Laplace operator.
The current result deals with self-adjointness of Stark operator on finite intervals. We give all parametrization giving self-adjointness. It should be stressed that the self-adjoint extensions of different domains are parameterized by a unitary group. The result is based on the von Neumann theory which provides necessary and sufficient conditions for the existence of self-adjoint extensions of closed symmetric operators in Hilbert space [32]. This theory is fully general and complectly solve the problem of self-adjoint extensions of every densely defined and closed symmetric operator in abstract Hilbert space using unitary operator between each deficiency [24]. However, for specific classes like stark operators, it would be suitable to have a more concrete characterization of self-adjoint extension. At section 4 some particular extensions are considered and spectral properties are given. We focus that, changing the self-adjoint extensions leads to different spectral results. The phenomena of splitting of degenerates eigenvalues is observed for some particular self-adjoint boundary conditions. In Section 4.1, we give more details on the subject of splitting phenomena. The energy spectrum is calculated using the stable-state schrodinger characterized by the specific potential structure with the constant electric field. The problem is solved by representing the eigen-

function as a superposition of the airy functions despite the potential is simple (square-well), which lead to an analytical solution for the equation transforming on a very computationally complexity. The problem overcame in many papers using perturbation method, we refer to [26] among others. This has the disadvantages (as any perturbation method) to be effective only for weak-enough electric field and produce invalid results for strong ones. For this, developing numerical methods to calculate the energy spectrum remains pertinent. It should be stressed that in one of our studied examples, our calculation confirm the experimental results (splitting phenomena). This method could lead to an exactly solvable approximate model.

2 The model and the result

We consider the Stark operator

$$H = -\frac{d^2}{dx^2} + Fx, F > 0. \tag{2}$$

The functional space is the Hilbert space $L^2([-L, L])$ equipped with the scalar product

$$\langle f, g \rangle = \int_{-L}^{L} f(x)\overline{g(x)}dx, \forall f, g \in L^2([-L, L]).$$

We notice that (2) corresponds to the (1), with $V(x) = 0$ if $x \in [-L, L]$ and $V(x) = +\infty$ if not.

This model corresponds to a particle in a box : $[-L, L]$ for $L > 0$ in a presence of an electric fled of strength F. From a mathematical standpoint the situation could be seen to be quite similar to the one with the free Laplacian, but up to our knowledge, it did not appear before in the literature. So we give details below.

The maximal domain in which H is well defined will denote by $\mathcal{D}_{max}$, i.e

$$\mathcal{D}_{max} = \{f \in L^2([-L, L]); Hf \in L^2([-L, L])\}.$$

Consider the domain

$$\mathcal{D}_0 = \{\psi \in \mathcal{D}_{max} \text{ and}, \psi(-L) = \psi(L) = 0 = \psi'(-L) = \psi'(L)\}.$$

It is a closed and densely defined operator. The density of $\mathcal{D}_0$ follows from the fact that $C_0^\infty([-L, L]) \subset \mathcal{D}_0$. The closeness of H is due to the fact that the maximal domain is considered. Moreover, using the density of $H^2([-L, L])$ in L^2, we can get the closeness property. Using integration by part we get that H is also a symmetric operator. The adjoint of H is $H^* = H$ and

$$\mathcal{D}(H^*) = \{\psi \in \mathcal{D}_{max} \text{ withount any other condition}\}.$$

Hence, H is not a self-adjoint operator on $\mathcal{D}_0$ and the considered domain is too small to be associated to aselfadjoint operator. So, H does not represent any physical observable and can not generate any physical dynamics.

Let us notice that in the case of bounded operators as the domain of a densely defined bounded operator can always be extended to the entire vector space, therefore, a bounded Hermitian operator is also self-adjoint. However, in the unbounded case the situation is pathological and a little bit more subtle.

Thus, we are interested clarifying conditions and domain under which symmetric, densely-defined H can be self-adjoint and to know its self-adjoint extensions.

Theorem 2.1. *Let H be the operator defined by (2). Then H has infinitely many self-adjoint extensions, these possible self-adjoint extensions of H are parameterized by a unitary matrix $U \in U(2)$. Let us denote them by $H_U = (H, \mathcal{D}(U))$, here $\mathcal{D}(U)$ is the space of functions $\phi \in \mathcal{D}_{max}$ satisfying the following boundary conditions*

$$\begin{pmatrix} L\phi'(-L) - i\phi(-L) \\ L\phi'(L) + i\phi(L) \end{pmatrix} = U \begin{pmatrix} L\phi'(-L) + i\phi(-L) \\ L\phi'(L) - i\phi(L) \end{pmatrix}. \tag{3}$$

Each self-adjoint extension has purely discrete spectrum.

The result of the last theorem could be related to the von Neumann theorem [32] which a powerful tool used in such situation. The proof of Theorem 2.1 is given in the next section.

3 Deficiency indices, von Neumann's theorem and self-adjoitness

First we recall the definition and some properties of deficiency indices. For a Hilbert space $\mathcal{H}$, and operator $(A, \mathcal{D}(A))$ defined on $\mathcal{H}$, with $\mathcal{D}$ a dense subspace of $\mathcal{D}$. The domain $\mathcal{D}(A^*)$, of the adjoint A^*, is the space of functions φ such that the linear form

$$\psi \to \langle A\varphi, \psi \rangle,$$

is continuous for the norm of $\mathcal{H}$. So there exists a $\psi^* \in \mathcal{H}$ such that

$$\langle A\varphi, \psi \rangle = \langle \varphi, \psi^* \rangle.$$

We define the adjoint A^* by $A^*\psi = \psi^*$ [28]. The space $\mathcal{E} = \mathcal{D}(A^*)/\mathcal{D}(A)$. Is called factor space.

Definition 3.1. *For a densely defined, symmetric and closed operator $(A, \mathcal{D}(A))$, we define the deficiency subspaces $\mathcal{D}_\pm$ by*

$$\mathcal{D}_+ = \{\varphi \in \mathcal{D}(A^*), A^*\varphi = z_+\varphi, Imz_+ > 0\},$$

$$\mathcal{D}_- = \{\varphi \in \mathcal{D}(A^*), A^*\varphi = z_-\varphi, Imz_- < 0\},$$

with respective dimensions d_+, d_-. These are called the deficiency indices of the operator A and will be denoted by the ordered pair (d_+, d_-).

We note that d_+ and d_- are independent of the points z_+ and z_- respectively [2, 6, 32], so for simplicity we take $z_+ = i$ and $z_- = -i$. The theorem below known as von Neumann theorem relates the deficiency indices to the number of self-adjoint extension of an operator for the proof see [2, 6, 32].

Theorem 3.2. *[32] For a symmetric and closed operator A with deficiency indices (d_+, d_-) there are three possibilities:*

1. *If $d_+ = d_- = 0$, then A is selfadjoint.*

2. *If $d_+ = d_- = d \geq 1$, then A has infinitely many self-adjoint extensions, parameterized by a unitary $d \times d$ matrix.*

3. *If $d_+ \neq d_-$, then A has no selfadjoint extension.*

4. *The dimension of the factor space is $d_- + d - +$.*

Remark 3.3. 1. *The first point of the last theorem is a necessary and sufficient condition.*

2. *The second point says that the set of all selfadjoint extensions is parameterized by d^2 real parameter.*

3. *The von Neumann's argument did not show how we construct such self-adjoint extensions.*

Let us consider the equation

$$H\psi(x) = \pm i\lambda_0 \psi(x),\ \lambda_0 > 0, \tag{4}$$

with H as in (2). This equation known as Airy equation has two independents solutions $Ai(\cdot)$ and $Bi(\cdot)$ both in $L^2(-L,L)$(See 10.4.1 in [1]). So the deficiency indices of H are (2,2) and we will show that the self-adjoint extensions are parameterized by a $U(2)$ matrices. By Theorem 3.2 we conclude that dimension of the factor space $\mathcal{E} = \mathcal{D}(H^*)/\mathcal{D}(H)$ is 4.

To study these self-adjoint extensions, we start by introducing the sesquilinear form, for $\phi, \psi \in \mathcal{D}_{max}$

$$\mathcal{B}(\phi,\psi) = \frac{1}{2i}(\langle H^*\phi, \psi\rangle - \langle \phi, H^*\psi\rangle).$$

$\mathcal{B}$ depends only on the boundary values of ϕ and ψ. When $\phi = \psi$ we get

$$\mathcal{B}(\phi,\phi) = \frac{1}{2i}(\phi'(L)\overline{\phi(L)} - \phi(L)\overline{\phi'(L)} - \phi'(-L)\overline{\phi(-L)} + \phi(-L)\overline{\phi'(-L)}).$$

Using parallelogram identity twice and the identities

$$\frac{1}{2i}(x\overline{y} - y\overline{x}) = \frac{1}{4}(|x+iy|^2 - |x-iy|^2);\ \forall x,y \in \mathbb{C},$$

and

$$2(x\overline{y} + y\overline{x}) = |x+y|^2 - |x-y|^2;\ \forall x,y \in \mathbb{C},$$

we get that:

$$\begin{aligned} 4L\mathcal{B}(\phi,\phi) \;&=\; \mid L\phi'(-L) - i\phi(-L)\mid^2 + \mid L\phi'(L) + i\phi(L)\mid^2 \\ &\quad - \mid L\phi'(-L) + i\phi(L)\mid^2 - \mid L\phi'(L) - i\phi(L)\mid^2 . \end{aligned} \tag{5}$$

It is not obvious to conclude from the equation (5). As the factor space is of dimension 4, the boundary form $\mathcal{B}$ can be identified to the following skew linear form with $\mathbb{C}^4$ equipped with the standard hermitian metric.

$$\mathcal{B} : \mathbb{C}^4 \to \mathbb{C}$$
$$Z = (z_1, z_2, z_3, z_4) \mapsto \frac{1}{2i}(z_1\overline{z_2} - z_2\overline{z_1} - z_3\overline{z_4} + z_4\overline{z_3}).$$

This could be written as

$$\mathcal{B}(Z,Z) = \langle \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix}, J\begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix}\rangle.$$

With

$$J = \frac{1}{2}\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{pmatrix} .$$

$$\mathcal{B}(Z,Z) = 0 \Leftrightarrow Z \perp JZ.$$

We set

$$P_+ = \frac{1}{2}I + J, P_- = \frac{1}{2}I - J.$$

So we get the following properties

$$J = \overline{J^t}, 4J^2 = I.$$

and

$$P_+^2 = P_+, P_-^2 = P_-, P_+ = P_+^*, P_- = P_-^*,$$
$$P_+P_- = 0, P_+ + P_- = I.$$

So P_+, P_- are orthogonal projectors. These matrices project the space $\mathbb{C}^4$ onto subspaces $\mathbb{C}_+^4 = P_+\mathbb{C}^4$ and $\mathbb{C}_-^4 = P_-\mathbb{C}^4$ and we get that

$$\mathbb{C}^4 = \mathbb{C}_+^4 \oplus \mathbb{C}_-^4.$$

It turns out that J-self-orthogonal subspaces of $\mathbb{C}^4$ are in one to one correspondence with unitary operators acting from $\mathbb{C}_+^4$ onto $\mathbb{C}_-^4$.
Let $\mathcal{D}$ be a domain such that

$$\mathcal{D}(H) \subseteq \mathcal{D} \subseteq \mathcal{D}(H^*).$$

To any $\mathcal{D}$ corresponds an extension of the operator H.

$$H_{\mathcal{D}}\phi = H^*\phi, \ \forall \phi \in \mathcal{D}.$$

We denote by $\mathcal{D}^{\perp J}$ the space

$$\{x \in \mathcal{E} : B(x,y) = 0, \ \forall y \in \mathcal{D}\}.$$

We have

$$(H_{\mathcal{D}})^* = H_{\mathcal{D}^{\perp J}}.$$

The domain of a self-adjoint extension of H is a subspace of $\mathcal{D}_{max}$, on which the sesquilinear form $\mathcal{B}(\phi,\phi)$ vanishes identically. So $H_{\mathcal{D}}$ is self-adjoint if only if

$$\mathcal{D} = \mathcal{D}^{\perp J}.$$

Below we show that these possible self-adjoint extensions of H are parameterized by a unitary matrix $U \in U(2)$.

Lemma 3.4. *1. Let U be an unitary operator acting from $\mathbb{C}_+^4$ onto $\mathbb{C}_-^4$. Then the subspace $\mathcal{D}_U = \{v + Uv, v \in \mathbb{C}_+^4\}$ is J-self-orthogonal, that is*

$$\mathcal{D}_U = \mathcal{D}_U^{\perp J}.$$

2. For very J-self-orthogonal subspace $\mathcal{D}$ of $\mathbb{C}^4$ there exists a unitary operator $U : \mathbb{C}_+^4 \to \mathbb{C}_-^4$ such that

$$\mathcal{D} = \mathcal{D}_U.$$

3. *The correspondence between J-self-orthogonal subspaces and unitary operators acting from $\mathbb{C}^4_+$ onto $\mathbb{C}^4_-$ is one to one;*

$$U_1 = U_2 \Leftrightarrow \mathcal{D}_{U_1} = \mathcal{D}_{U_2}.$$

Proof. 1. The mapping from $\mathbb{C}^4_+$ to $\mathcal{D}_U$ defined by $v \mapsto v + Uv$, is one to one. Indeed, the equality $v + Uv = 0$ implies that $\| v \| = 0$ as v is orthogonal to $Uv \in \mathbb{C}^4_-$. So the mapping is bijective and we get

$$dim(\mathcal{D}_U) = dim(C^4_+) = 2.$$

Let v_1 and v_2 be two arbitrary vectors of $\mathbb{C}^4_+$. We set $u_1 = v_1 + Uv_1$ and $u_2 = v_2 + Uv_2$. As $2J = P_+ - P_-$ and $v_i = P_+ v_i$, $Uv_i = P_- Uv_i, i = 1,2$ using the properties of P_+ and P_-, we get that u_1 and u_2 are J orthogonal. So

$$\mathcal{D}_U \subseteq (\mathcal{D}_U)^{\perp J}.$$

Since the Hermitian form $\mathcal{B}$, is non-degenerate on $\mathbb{C}^4$, then $dim(\mathcal{D}_U^{\perp J}) = dim\mathbb{C}^4 - dim(\mathcal{D}_U) = 2$. So

$$\mathcal{D}_U = (\mathcal{D}_U)^{\perp J},$$

i.e the subspace $\mathcal{D}_U$ is J-self-orthogonal.

2. Let $\mathcal{D}$ be a J-self-orthogonal subspace. If

$$v \in \mathcal{D}, v = v_1 + v_2, v_1 \in \mathbb{C}^4_+, v_2 \in \mathbb{C}^4_-,$$

the the condition of J self-orthogonality; $v \perp_J v$ means that $\langle v_1, v_1 \rangle = \langle v_2, v_2 \rangle$. So, if $v_1 = 0$, the also v. This implies that the projection mapping $v \to P_+ v$, considered as a mapping from $\mathcal{D} \to \mathbb{C}^4_+$ is injective. For a J-self-orthogonal subspace $\mathcal{D}$ of $\mathbb{C}^4$. The equality $dim(\mathcal{D}) = dim(\mathbb{C}^4) - dim(\mathcal{D})$ holds. So $dim(\mathcal{D}) = dim(\mathbb{C}^4_+)$ So, the injective linear mapping $v \to P_+ v$ is surjective . The inverse mapping defined from $\mathbb{C}^4_-$ is presented in the form $v = v_1 + Uv_1$, with U is a unitary operator acting from $\mathbb{C}^+_4$ into $\mathbb{C}^4_-$. This mapping $v_1 \to v_1 + Uv_1$ maps the space $\mathbb{C}^4_+$ onto the subspace $\mathcal{D}$.
As $\langle v, Jv \rangle = 0$ then $\langle v_1, v_1 \rangle = \langle v_2, v_2 \rangle$, with $v_2 = Uv_1$. As $v_1 \in \mathbb{C}^4_+$ is arbitrary, this means that the operator U is isometric. Since $dim\mathbb{C}^4_+ = dim\mathbb{C}^4_-$ the operator is unitary. Thus, the originally given J-self-orthogonal subspace $\mathcal{D}$ is of the form $\mathcal{D}_U$. With U is a unitary operator acting from $\mathbb{C}^4_+$ to $\mathbb{C}^4_-$.

3. The equality $\mathcal{D}_{U_1} = \mathcal{D}_{U_2}$ means that any vector of the form $v_1 + Uv_1$ where $v_1 \in \mathbb{C}^4_+$ can be represented in the form $v_2 + Uv_2$ with some $v_2 \in \mathbb{C}^4_+$:

$$v_1 + U_1 v_1 = v_2 + U_2 v_2.$$

As $v_1, v_2 \in \mathbb{C}^4 - +, U_1 v_1, U_2 v_2 \in \mathbb{C}^4_-$, then $v_1 = v_2$ and $U_1 v_1 = U_2 v_1$ for any $v_1 \in \mathbb{C}^4_+$ which means that $U_1 = U_2$. Thus

$$\mathcal{D}_{U_1} = \mathcal{D}_{U_2} \Rightarrow U_1 = U_2.$$

This ends the proof of Lemma 3.4. □

Now we return to the equation (5) with boundary condition by setting $z_1 = L\phi'(-L) - i\phi(-L), z_2 = L\phi'(L) + i\phi(L), z_3 = L\phi'(-L) + i\phi(-L)$ and $z_4 = L\phi'(L) - i\phi(L)$ .Let us denote them by $H_U = (H, \mathcal{D}(U))$, here $\mathcal{D}$(U) is the space of functions $\phi \in \mathcal{D}_{max}$ satisfying by (5), the following boundary conditions

$$\begin{pmatrix} L\phi'(-L) - i\phi(-L) \\ L\phi'(L) + i\phi(L) \end{pmatrix} = U \begin{pmatrix} L\phi'(-L) + i\phi(-L) \\ L\phi'(L) - i\phi(L) \end{pmatrix}. \tag{6}$$

These boundary conditions describe all the self-adjoint extensions $(H_U, \mathcal{D}(U))$ of H.

Remark 3.5. *Let us point that the boundary condition (6) is so important and could even break parity properties of solutions of eigenfunctions equations and even in the case when the potential is of definite parity we can't say noting about the solutions.*

Using the fact that for n order differential operator with deficiency indices (n, n) all of its self-adjoint extensions have a discrete spectrum, we conclude that all the spectra of the H_U are totaly discrete. So the proof of Theorem 2.1 is ended. □

For completeness let us recall that a 2×2 matrix U with complexes coefficients is an element of $U(2)$ if and only if $U^* \cdot U = I_2$. So the determinant of U is a complex of modulus 1 and $detM : U(2) \to U(1)$ is a group homomorphism which is surjective and having the subgroup $SU(2)$ of matrices determinant one as a kernel. So

$$U(1) \cong U(2)/SU(2).$$

By this we get the following parametrization of $U(2)$ and write that

$$U = e^{i\theta} M, \; detM = 1, i.e \; M \in SU(2). \tag{7}$$

For this let us recall some results and properties of $SU(2)$, representation.

3.1 Representation and topology of $SU(2)$

As we deal with matrices of order two there is more explicit properties. Let $M \in SU(2)$

$$M = \begin{pmatrix} \alpha & \beta \\ \gamma & \lambda \end{pmatrix}; M^* = \begin{pmatrix} \overline{\alpha} & \overline{\gamma} \\ \overline{\beta} & \overline{\lambda} \end{pmatrix}; \tag{8}$$

using the fact $det(M) = \alpha\beta - \beta\gamma = 1$, we get

$$M^{-1} = \begin{pmatrix} \lambda & -\beta \\ -\gamma & \alpha \end{pmatrix}. \tag{9}$$

So

$$M^{-1} = M^* \Leftrightarrow \lambda = \overline{\alpha}; \text{ and } \; \gamma = -\overline{\beta},$$

and the generic form of matrices of $SU(2)$ is given by the following parametrization

$$M = \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix}; |\alpha|^2 + |\beta|^2 = 1. \tag{10}$$

By taking $\alpha = \alpha_1 + i\alpha_2$ and $\beta = \beta_1 + i\beta_2, \alpha_i, \beta_i \in \mathbb{R}$, we get that

$$|\alpha_1|^2 + |\alpha_2|^2 + |\beta_1|^2 + |\beta_2|^2 = 1.$$

This gives that $SU(2)$ as a topological space is holomorphic to the sphere unity S^3 in $\mathbb{R}^4$. $SU(2)$ has three generators given Pauli matrices [30].

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{11}$$

We write

$$M = \alpha_1 I_2 - i(\alpha_2, \beta_1, \beta_2).(\tau_1, \tau_2, \tau_3).$$

3.2 Form of solutions

The spectral equation associated to stark operator has been solved by Airy special functions $Ai(\cdot)$ and $Bi(\cdot)$ [13, 33], see Figures 1, which are the solution of the following second order differential equation

$$-\frac{d^2\psi}{dx^2}(x) + Fx\psi(x) = E\psi(x). \tag{12}$$

Using the change of variable:

$$\xi = \frac{E}{F\rho}; \rho = F^{-\frac{1}{3}},\ x = \rho z,$$

we get the new equation

$$\psi''(z) = (z - \xi)\psi(z). \tag{13}$$

The solutions of equ. (12) are two linearly independent Airy functions $Ai(z-\xi)$ and $Bi(z-\xi)$. The eigenfunctions associated to the equation (13) are given as a superposition of two linearly independent functions of the form

$$\phi(z) = A \cdot Ai(z - \xi) + B \cdot Bi(z - \xi);\ \mathbf{\Phi} = \begin{pmatrix} A \\ B \end{pmatrix} \in \mathbb{R}^2. \tag{14}$$

Remark 3.6. *At this stage, lets remark that works dealing with a half line domaine, i.e, with a potential $V(x) = 0$ for $x \geq 0$ and $V(x) = +\infty$ for $x < 0$; in (14) we get just $Ai(\cdot)$ and the quantized energies are then given in terms of the zeros of the well-behaved Airy $Ai(\cdot)$. So the eigenvalues of the operator are given by $E = F^{\frac{2}{3}}\xi$, with $-\xi$ are the k-th zero of Ai.*

The solutions of equation (13) are of the form

$$\phi(x) = A \cdot Ai(F^{\frac{1}{3}}(x - \frac{E}{F})) + B \cdot Bi(F^{\frac{1}{3}}(x - \frac{E}{F})). \tag{15}$$

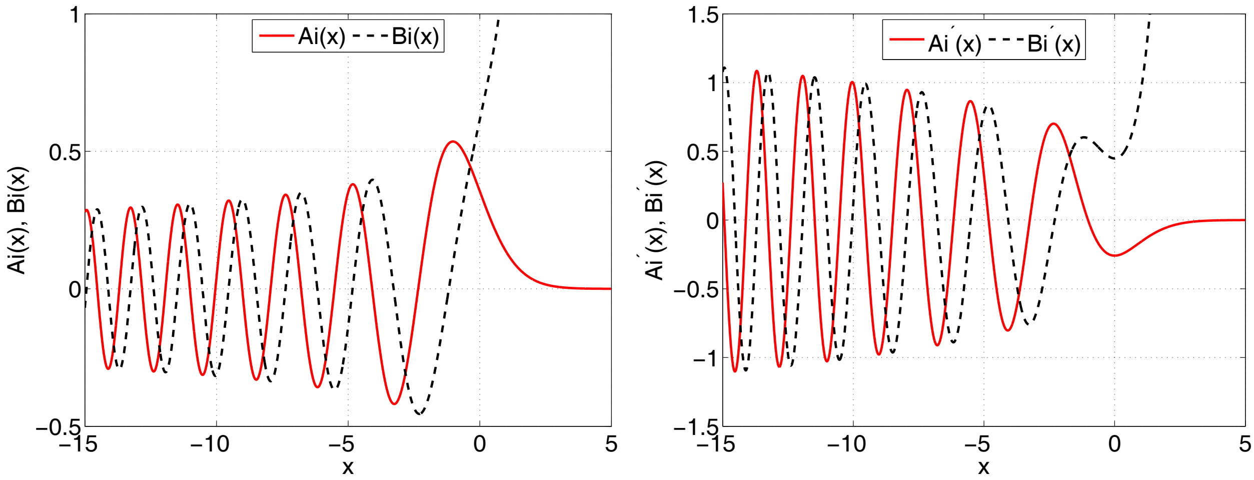


Figure 1: Airy functions and the corresponding derivatives.

We set

$$L^{+}(E,F) = F^{\frac{1}{3}}(L-\frac{E}{F}), \tag{16}$$

and

$$L^{-}(E,F) = -F^{\frac{1}{3}}(L+\frac{E}{F}). \tag{17}$$

So

$$\begin{aligned}
&\begin{pmatrix} L\phi'(-L)-i\phi(-L) \\ L\phi'(L)+i\phi(L) \end{pmatrix} \\
=& \begin{pmatrix} L(A\cdot Ai'(L^{-}(E,F))+B\cdot Bi'(L^{-}(E,F)))-i(A\cdot Ai(L^{-}(E,F))+B\cdot Bi(L^{-}(E,F))) \\ L(A\cdot Ai'(L^{+}(E,F))+B\cdot Bi'(L^{+}(E,F)))+i(A\cdot Ai(L^{+}(E,F))+B\cdot Bi(L^{+}(E,F))) \end{pmatrix} \\
=& \begin{pmatrix} A(L\cdot Ai'(L^{-}(E,F))-iAi(L^{-}(E,F)))+B(L\cdot Bi'(L^{-}(E,F))-iBi(L^{-}(E,F))) \\ A(L\cdot Ai'(L^{+}(E,F))+iAi(L^{+}(E,F)))+B(L\cdot Bi'(L^{+}(E,F))+iB\cdot Bi(L^{+}(E,F))) \end{pmatrix} \\
=& \mathcal{L}(\xi)\mathbf{\Phi}.
\end{aligned}$$

With

$$\mathcal{L}(\xi) = \begin{pmatrix} L\cdot Ai'(L^{-}(E,F))-iAi(L^{-}(E,F)) & L\cdot Bi'(L^{-}(E,F))-iBi(L^{-}(E,F)) \\ L\cdot Ai'(L^{+}(E,F))+iAi(L^{+}(E,F)) & L\cdot Bi'(L^{+}(E,F))+iBi(L^{+}(E,F)) \end{pmatrix}.$$

and

$$\begin{aligned}
&\begin{pmatrix} L\phi'(-L)+i\phi(-L) \\ L\phi'(L)-i\phi(L) \end{pmatrix} \\
=& \begin{pmatrix} A(L\cdot Ai'(L^{-}(E,F))+iAi(L^{-}(E,F)))+B(L\cdot Bi'(L^{-}(E,F))+iBi(L^{-}(E,F))) \\ A(L\cdot Ai'(L^{+}(E,F))-iAi(L^{+}(E,F)))+B(L\cdot Bi'(L^{+}(E,F))-iB\cdot Bi(L^{+}(E,F))) \end{pmatrix} \\
=& \mathcal{M}(\xi)\mathbf{\Phi}.
\end{aligned}$$

With

$$\mathcal{M}(\xi) = \begin{pmatrix} L\cdot Ai'(L^{-}(E,F))+iAi(L^{-}(E,F)) & L\cdot Bi'(L^{-}(E,F))+iBi(L^{-}(E,F)) \\ L\cdot Ai'(L^{+}(E,F))-iAi(L^{+}(E,F)) & L\cdot Bi'(L^{+}(E,F))-iBi(L^{+}(E,F)) \end{pmatrix}.$$

Using (6) we get the following relation between $\mathcal{L}(\xi)$ and $\mathcal{M}(\xi)$.

$$(\mathcal{L}(\xi) - U\mathcal{M}(\xi))\mathbf{\Phi} = 0. \tag{18}$$

To get a nontrivial solution to (14), we need that $(\mathcal{L}(\xi) - U\mathcal{M}(\xi))$ be not invertible which is equivalent to

$$det(\mathcal{L}(\xi) - U\mathcal{M}(\xi)) = 0. \tag{19}$$

Unfortunately it is not possible to get a simple analytic expression for the equation (19). Below, we give some particular cases which allow us to simplify least a little bit the general expression.

4 Interesting particular cases

In this section, we consider four particular cases of U. They are the most interesting and generally studied in literature [20, 23, 28, 33], known as Dirichlet, Neumann, Dirichlet-Neumann conditions and others. In general, it is not trivial to solve explicitly the determinant equations (19). In [13], the authors used numerical methods. Namely, the classical "Newton method" in "Mathematica tools" by "Find Root". Here, we implement a combination of the Bisection and the Newton methods. We approximate the zeros of the determinants with a maximal error 10^{-8}. Below, we consider some particular cases, which allow us to perform interesting computational results. For a fixed interval length L, we compute the first four eigenvalues for different fields F. Thereafter, for fixed F, we determined the first four eigenvalues for different width L of the quantum well. The associated eigenfunctions are also plotted.

1. The case $U = I$.

   This case leads to the operator $H_I = (H, \mathcal{D}(I))$ known as Dirichlet operator, with

   $$\{\phi \in L^2([-L,L]), H_{I_2}\phi \in L^2([-L,L]) \text{ and } \phi(-L) = \phi(L) = 0\}. \tag{20}$$

   So

   $$\mathcal{L}(\xi) - U\mathcal{M}(\xi) = \mathcal{L}(\xi) - \mathcal{M}(\xi) = 2i\begin{pmatrix} -Ai(L^-(E,F)) & -Bi(L^-(E,F)) \\ Ai(L^+(E,F)) & Bi(L^+(E,F)) \end{pmatrix}.$$

   The equation (19) yields to

   $$Ai(L^-(E,F))Bi(L^+(E,F)) - Ai(L^+(E,F))Bi(L^-(E,F)) = 0. \tag{21}$$

   To get the representation of the eigenfunction $\phi_n(x)$ associated to the eigenvalue E_n already calculated and given in table 1. We use the equation (14) and the boundary conditions given in (20) to obtain

   $$A \cdot Ai(L^+(E,F)) + B \cdot Bi(L^+(E,F)) = 0, \tag{22}$$

   and

   $$A \cdot Ai(L^-(E,F)) + B \cdot Bi(L^-(E,F)) = 0. \tag{23}$$

This gives that that

$$A = -B\frac{Bi(L^-(E,F))}{Ai(L^-(E,F))} = -B\frac{Bi(L^+(E,F))}{Ai(L^+(E,F))}.$$

So finally, we get that

$$\phi_n(x) = C\big[Bi(L^-(E,F)) \cdot Ai(F^{\frac{1}{3}}(x - \frac{E_n}{F})) - Ai(L^-(E,F)) \cdot Bi(F^{\frac{1}{3}}(x - \frac{E_n}{F}))\big], \quad (24)$$

with $C \in \mathbb{R}$ and

$$L^+(E,F) = F^{\frac{1}{3}}(L - \frac{E}{F}) \qquad \text{and} \qquad L^-(E,F) = -F^{\frac{1}{3}}(L + \frac{E}{F}). \quad (25)$$

In table 1, we give the eigenvalues for different cases. It should be stressed that an interesting effect appears by varying L and F. In the Figures 3. and 4., respectively, we plot the corresponding eigenfunctions for different values of L and F.

L	F	E_1	E_2	E_3	E_4
1	0	2.4674	9.8696	22.2066	39.4784
1	0.01	2.4673	9.8696	22.2066	39.4784
1	0.1	2.4672	9.86965	22.2066	39.4784
1	1	2.4498	9.8748	22.2097	39.4803
1	5	2.0416	9.9877	22.2841	39.5261
1	1	2.4498	9.8748	22.2097	39.4803
2	1	0.3554	2.5324	5.6007	9.9001
3	1	−0.6618	1.0947	2.6628	4.5376
4	1	−1.6618	0.0879	1.5216	2.8152

Table 1: Eigenvalues of the case 1

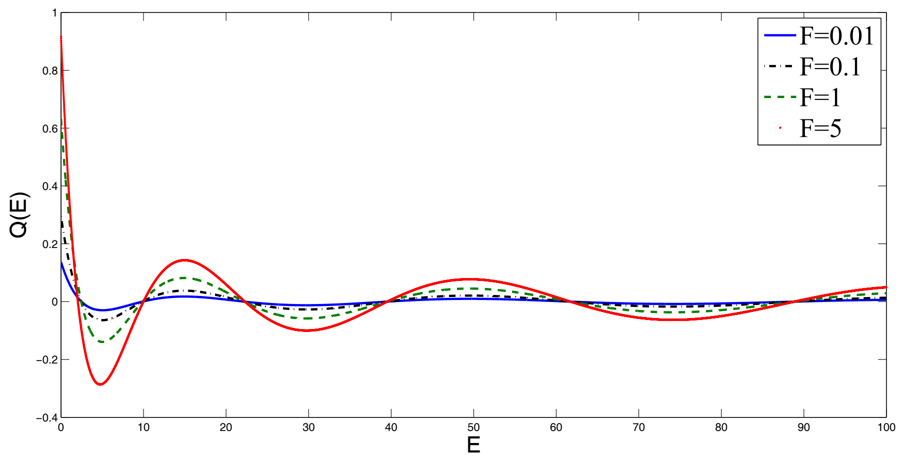
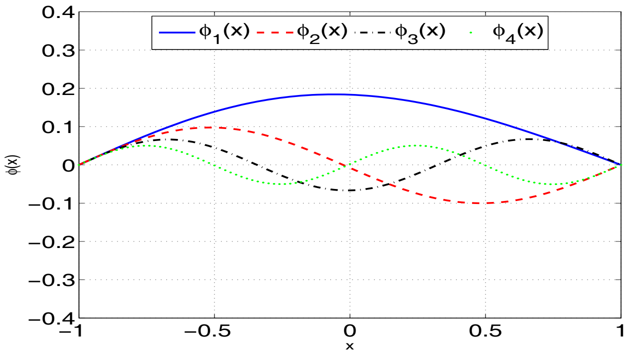
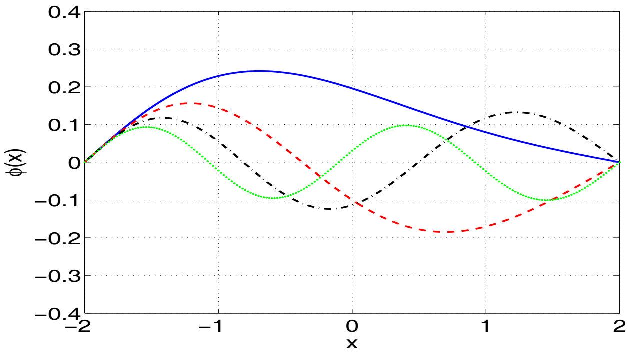


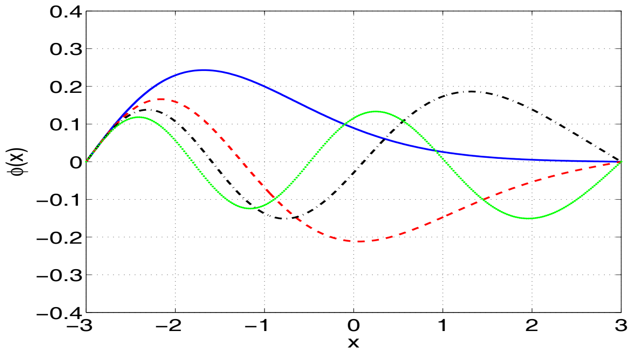
Figure 2: Determinant of case 1.



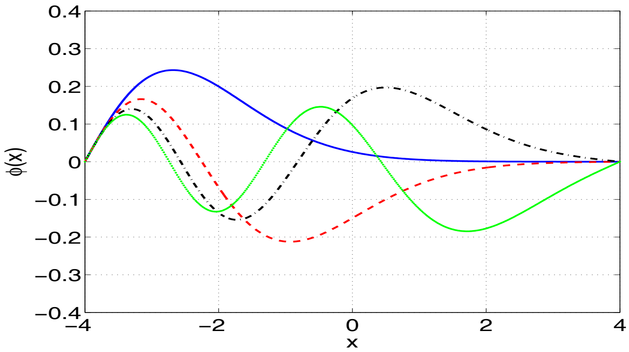
(a) $L=1$, $F=1$



(b) $L=2$, $F=1$

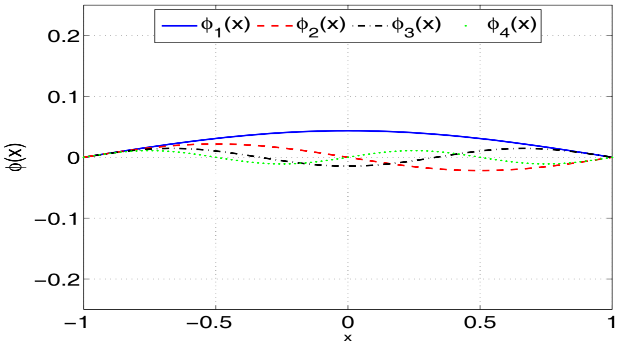


(c) $L=3$, $F=1$

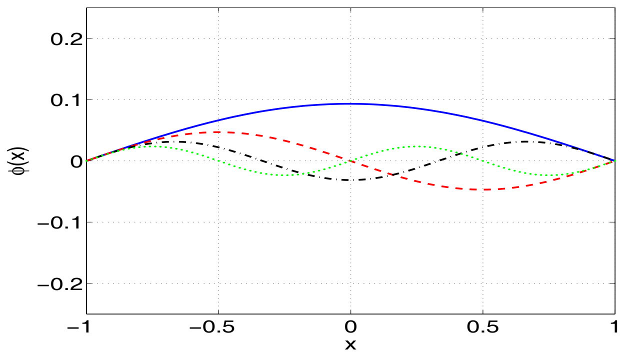


(d) $L=4$, $F=1$

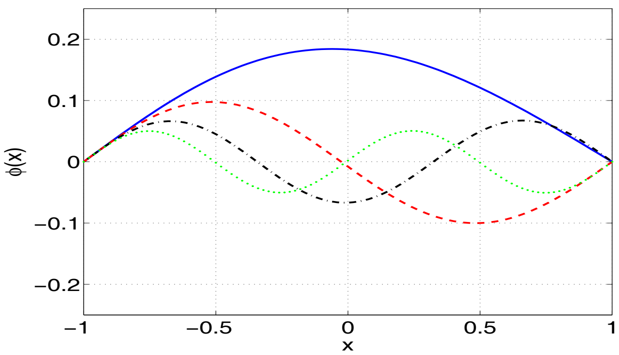
Figure 3: Case 1,F=1, L=1,2, 3, 4.



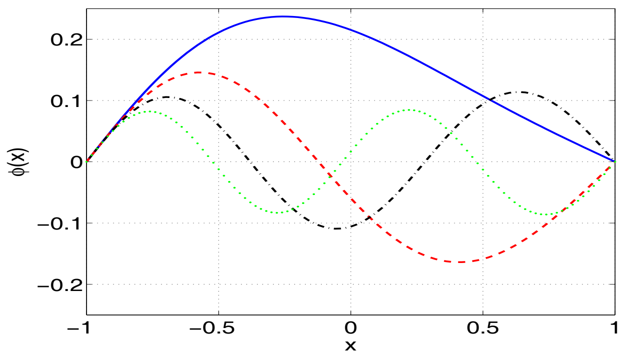
(a) $L=1,\ F=0.01$



(b) $L=1,\ F=0.1$



(c) $L=1,\ F=1$



(d) $L=1,\ F=5$

Figure 4: Case 1, L=1, F=0.01, 0.1, 1, 5.

2. The case $U=-I$.

   This particular case leads to the operator $H_{-I}=(H,\mathcal{D}(-I))$ known as Neumann operator, with

$$\{\phi\in L^2([-L,L]), H_U\in L^2([-L,L]) \text{ and } \phi'(-L)=\phi'(L)=0\}. \qquad (26)$$

   So

$$\mathcal{L}(\xi)-U\mathcal{M}(\xi)=\mathcal{L}(\xi)+\mathcal{M}(\xi)=2L\begin{pmatrix} Ai'(L^-(E,F)) & Bi'(L^-(E,F)) \\ Ai'(L^+(E,F)) & Bi'(L^+(E,F)) \end{pmatrix}.$$

   The equation (19) yields to

$$Ai'(L^-(E,F))Bi'(L^+(E,F))-Ai'(L^+(E,F))Bi'(L^-(E,F))=0. \qquad (27)$$

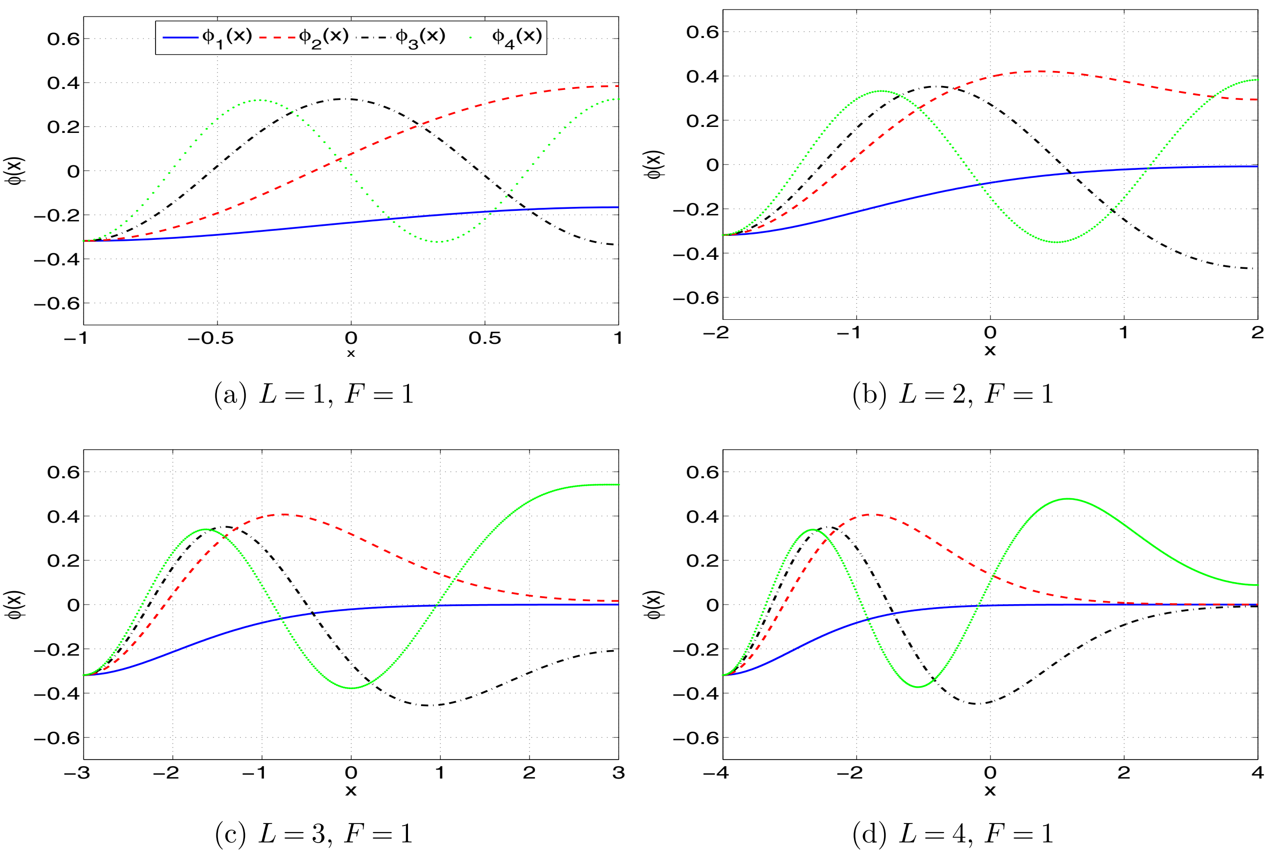
   For the eigenfunctions we get:

$$\phi_n(x)=C\left[Bi'(L^-(E,F))\cdot Ai(F^{\frac{1}{3}}(x-\frac{E_n}{F}))-Ai'(L^-(E,F))\cdot Bi(F^{\frac{1}{3}}(x-\frac{E_n}{F}))\right], \qquad (28)$$

   In the Figures 5. and 6., respectively, we plot the corresponding eigenfunctions related to case 2. for different values of L and F.

L	F	E_1	E_2	E_3	E_4
1	0	0	2.4674	9.8696	22.2066
1	0.01	-0.00001	2.4674	9.8696	22.2066
1	0.1	-0.0013	2.4684	9.8697	22.2066
1	1	-0.1278	2.5674	9.8825	22.2125
1	5	-2.0330	3.7841	10.215	22.3241
1	1	-0.1278	2.5674	9.8825	22.2112
2	1	-0.9818	1.1254	2.7014	5.6284
3	1	-1.9812	0.2475	1.7735	2.9509
4	1	-2.9812	-0.7518	0.8199	2.1551

Table 2: Eigenvalues of the case 2



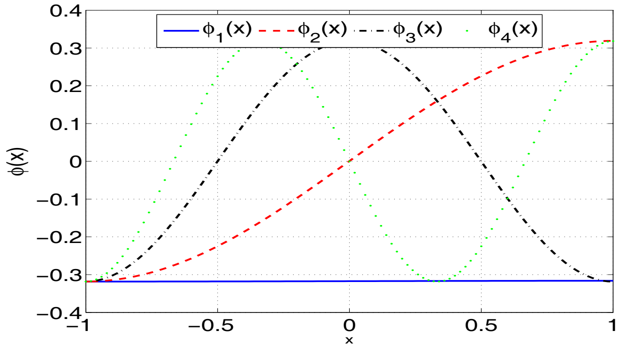
(a) $L = 1,\ F = 1$

(b) $L = 2,\ F = 1$

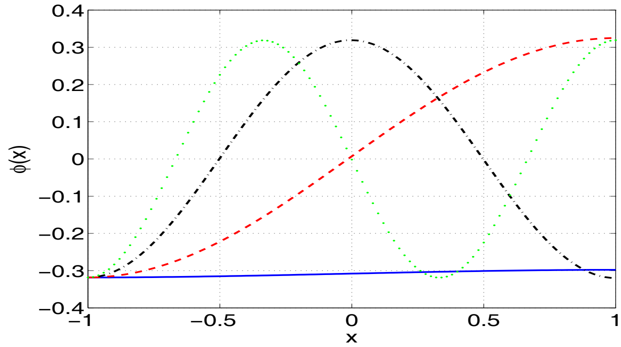
(c) $L = 3,\ F = 1$

(d) $L = 4,\ F = 1$

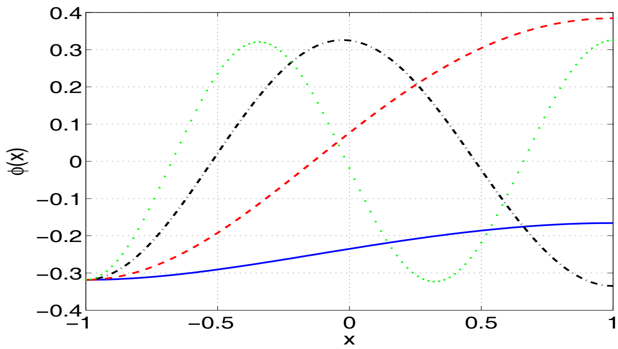
Figure 5: Case 2, F=1, L=1,2, 3, 4.



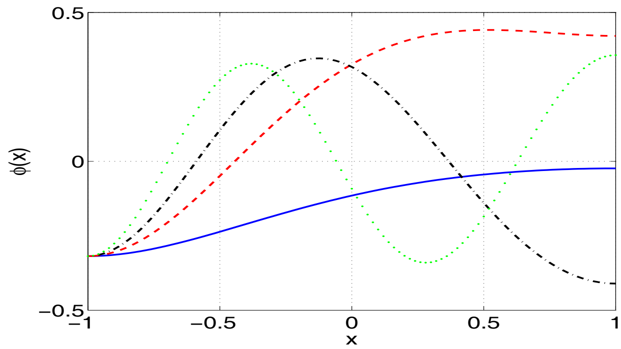
(a) $L=1,\ F=0.01$



(b) $L=1,\ F=0.1$



(c) $L=1,\ F=1$



(d) $L=1,\ F=5$

Figure 6: Case 2, L=1, F=0.01, 0.1, 1, 5.

3. The case $U=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$.

$$\{\phi\in L^2([-L,L]), H_U\in L^2([-L,L]) \text{ and } \phi(-L)=\phi'(L)=0\}. \tag{29}$$

In this particular case we get

$$\mathcal{L}(\xi)-U\mathcal{M}(\xi)=2\begin{pmatrix}-iAi(L^-(E,F)) & -iBi(L^-(E,F))\\ LAi'(L^+(E,F)) & LBi'(L^+(E,F))\end{pmatrix}.$$

The equation (19) yields to

$$Ai'(L^+(E,F))Bi(L^-(E,F))-Ai(L^-(E,F))Bi'(L^+(E,F))=0. \tag{30}$$

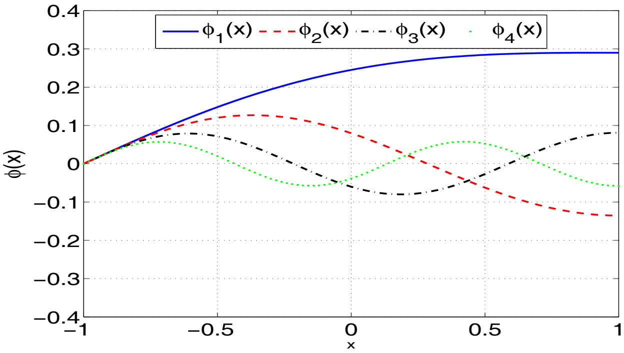
For the eigenfunctions we get that

$$\phi_n(x)=C\left[Bi(L^-(E,F))\cdot Ai(F^{\frac{1}{3}}(x-\frac{E_n}{F}))-Ai(L^-(E,F))\cdot Bi(F^{\frac{1}{3}}(x-\frac{E_n}{F}))\right], \tag{31}$$

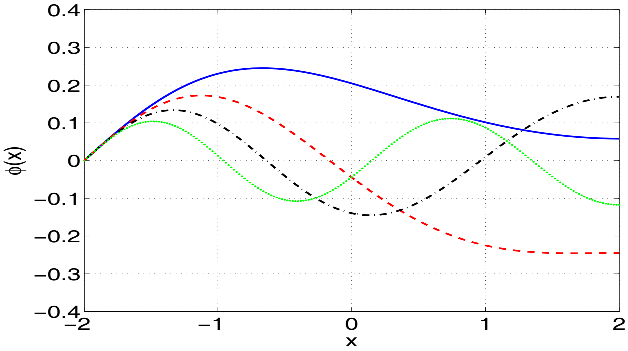
Similarly to the previous cases, we plot In the Figures 7. and 8., respectively, the eigenfunctions related to case 3. for different values of L and F.

L	F	E_1	E_2	E_3	E_4
1	0	0.6168	5.5516	15.4212	30.2256
1	0.01	0.6208	5.5521	15.4214	30.2257
1	0.1	0.6570	5.5563	15.4229	30.2265
1	1	0.9864	5.6153	15.4432	30.2367
1	5	1.6096	6.3689	15.6591	30.3396
1	1	0.9864	5.6153	15.4432	30.2367
2	1	0.3175	1.8336	3.9959	7.6204
3	1	−0.6619	1.0798	2.3777	3.6819
4	1	−1.6618	0.0879	1.5192	2.7497

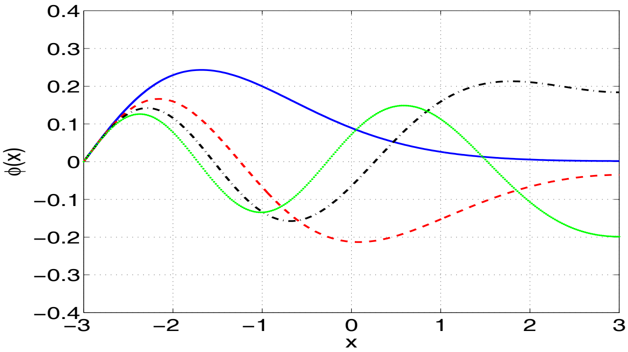
Table 3: Eigenvalues of the case 3



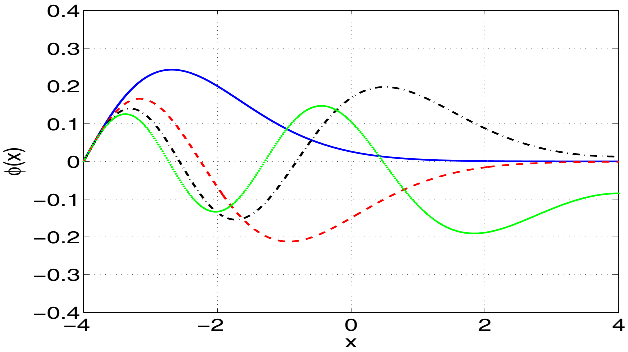
(a) $L=1,\ F=1$



(b) $L=2,\ F=1$

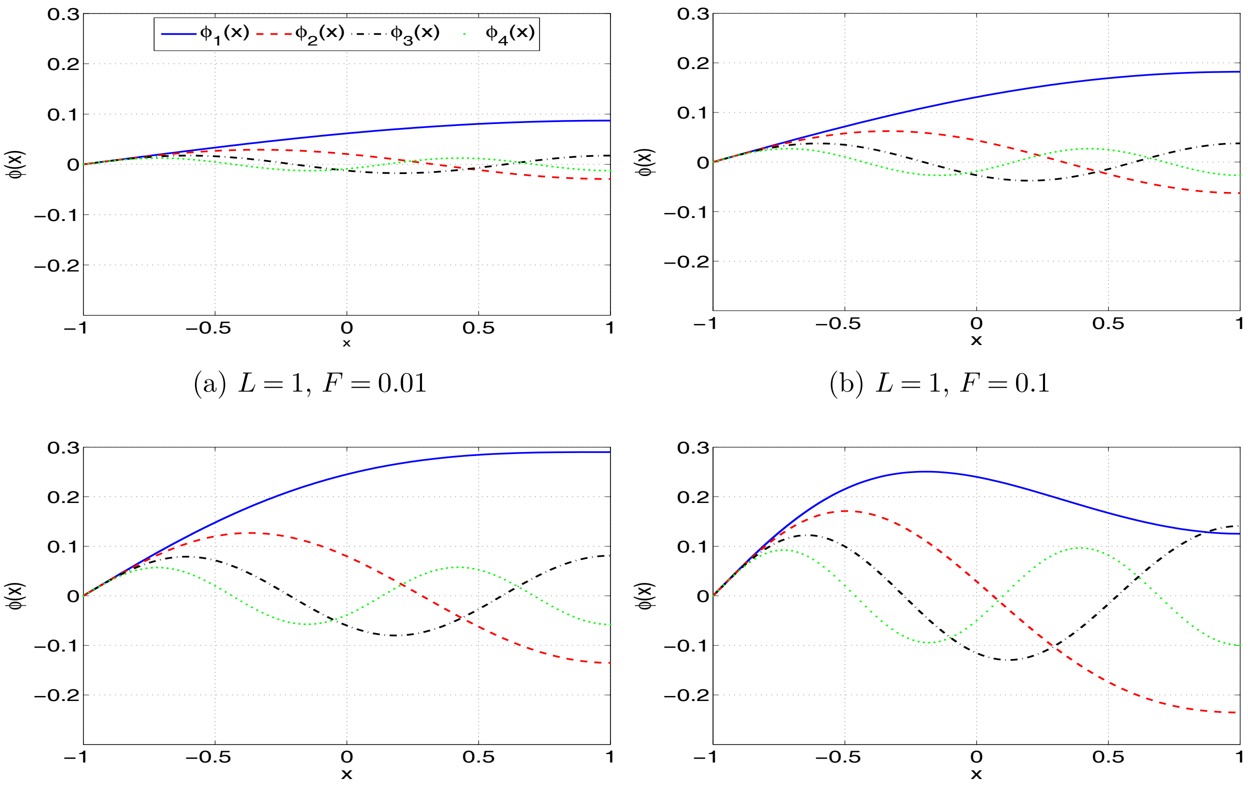


(c) $L=3,\ F=1$



(d) $L=4,\ F=1$

Figure 7: Case 3, F=1, L=1,2, 3, 4.



(a) $L = 1,\ F = 0.01$ (b) $L = 1,\ F = 0.1$

(c) $L = 1,\ F = 1$ (d) $L = 1,\ F = 5$

Figure 8: Case 3, L=1, F=0.01, 0.1, 1, 5.

Remark 4.1. *The absence of splitting and the shift phenomena in the non-degenerates case found in the previous three cases corresponds to the vanishing of the linear stark effect in the perturbation theory.*

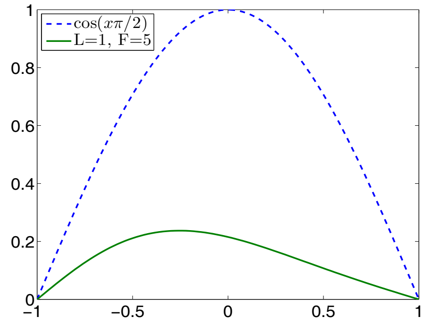
Remark 4.2. *It is important to note that, for the three previous cases, the eigenvalues decreases when L increases. This behavior is similar to the free case. See tables 1, 2 and 3. In figure 9, we remark that in the three cases, we have concentration of the eigenfunction on the left of the well when $F \neq 0$. i.e the particle is shifted to the left to minimize the total energy.*

4.1 Splitting phenomena

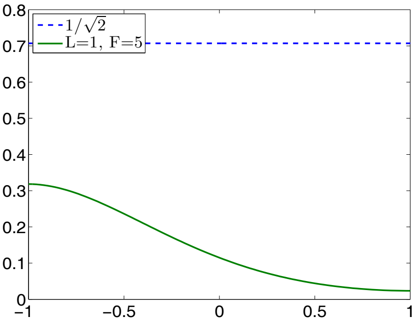
In this subsection, we will consider the case where $U = \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. It leads to the operator $H_{\tau_1} = (H, \mathcal{D}(\tau_1))$, with

$$\mathcal{D}(\tau_1) = \{\phi \in L^2([-L,L]), H_U \in L^2([-L,L]) \text{ and } \phi'(-L) = \phi'(L), \phi(L) = \phi(-L)\}. \quad (32)$$

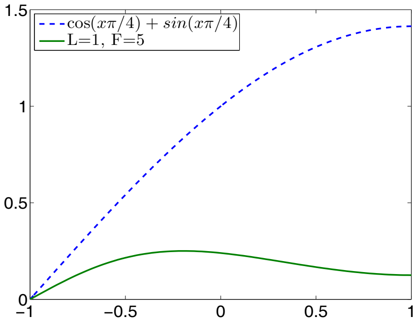
This case is not considered in literature. We shad some lights on the spectral theory on H_U. We expect it modeled the system which highlights the phenomena of splitting that is long sought by physician. Let's recall that since 1913, J. Stark stated that, when a particle is



(a) Case 1



(b) Case 2



(c) Case 3

Figure 9: Comparing the analytical eigenfunction for $L = 1,\ F = 0$ to the computational result for $L = 1,\ F = 5$.

exited a strong electric field splits on number of components an effect that goes after his name. The observed splitting agree with the calculation developed in this work. Which confirm the accuracy of the implemented numerical methods used here. The splitting is symmetrical in the where the field $F = 0$, see Figure 11.

Mathematically there is a deep relation between degeneracy and symmetry. This implies the existence of conjugation under which the operator remains unchanged. Such question is related to the theory of the symmetry group of the operator. The possible degeneracies of the eigenvalues with a particular symmetry group of the operator is specified by dimensionality of the irreducible representation of the group. The eigenfunction corresponding to m-degenerates eigenvalues form a basis for a m-dimensional irreducible representation of the symmetry group of the operator.

The degeneracy could arises due to the presence of some kind of symmetry in the system under consideration or related a characteristic of dynamical symmetry of the system. It also could be connected to the existence of bound orbits in the classical physics. The degeneracy in the present case is abolished when the symmetry is bracken by the presence of external electric field F. This engender the splitting in the degenerate energy level accrurating the numerical part of the proved result. We notes that the first order Stark effect is zero for the ground state (like Hydrogen atom).

The equation (19) yields to

$$[(Ai'(L^-(E,F)) - Ai'(L^+(E,F))(Bi(L^+(E,F)) - Bi(L^-(E,F))] \\ - [(Ai(L^+(E,F)) - A(L^-(E,F))(Bi'(L^-(E,F)) - Bi'(L^+(E,F))] = 0.$$

For the eigenfunctions, we get that

$$\begin{aligned} \phi_n(x) &= C\big[(Bi'(L^+(E,F)) - Bi'(L^-(E,F)))\cdot Ai(F^{\frac{1}{3}}(x-\frac{E_n}{F})) \\ &\quad +(Ai'(L^-(E,F)) - Ai'(L^+(E,F)))\cdot Bi(F^{\frac{1}{3}}(x-\frac{E_n}{F}))\big], \end{aligned} \tag{33}$$

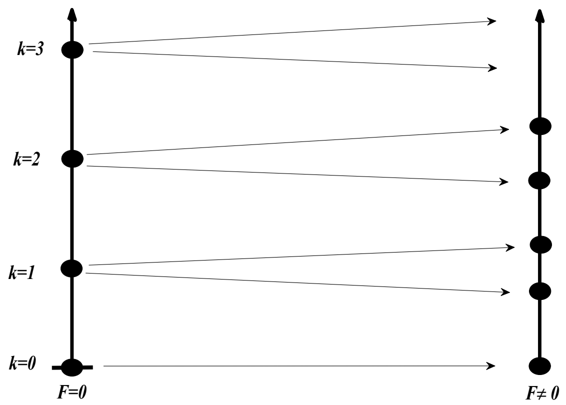
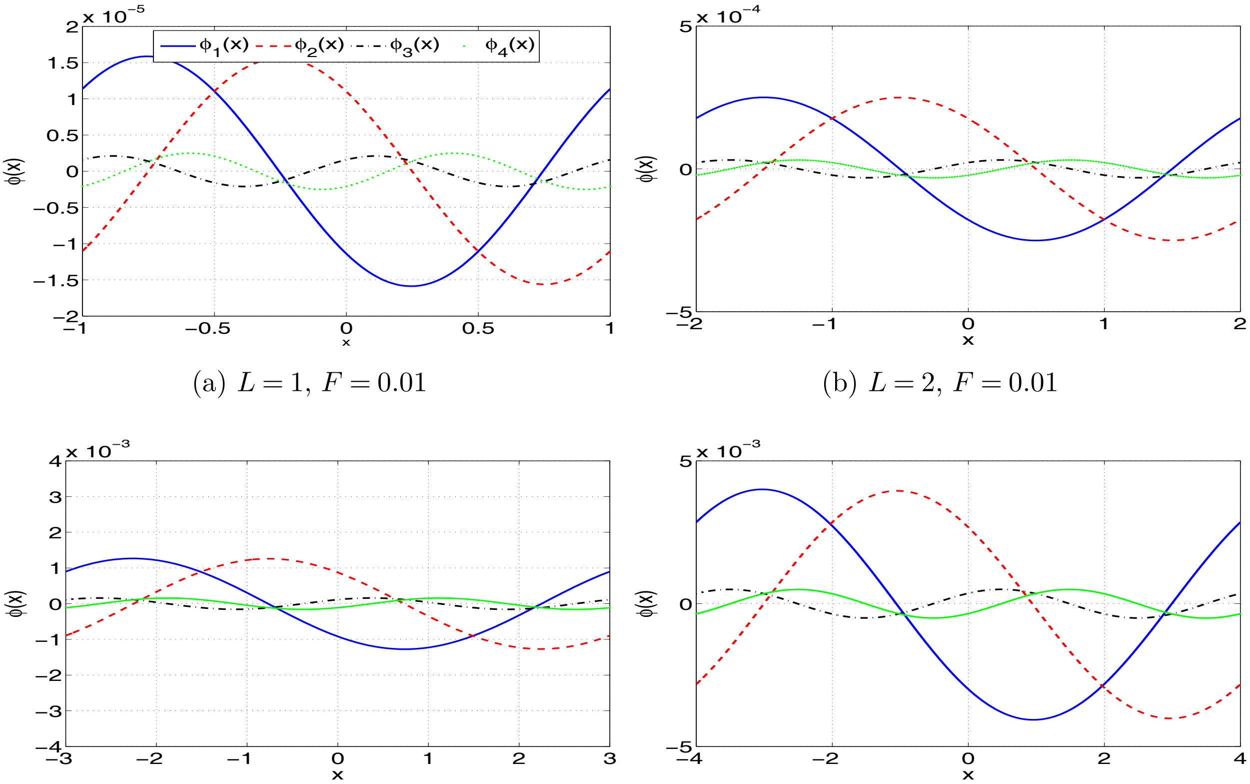


Figure 10: Splitting: Compared with other three cases. It is a non-degenerates eigenvalues and the stark effect was a shift of eigenvalues. In the current case it is degenerate and splitting.

L	F	E_0	E_1	E_2	E_3	E_4
1	0	0.0	9.8696	39.4784	$--$	$--$
1	0.01	0.0	9.86796	9.87119	39.4778	39.47891
2	0.01	0.0	2.46422	2.47705	9.86800	9.87119
3	0.01	0.0	1.09189	1.10144	4.34411	4.38889
4	0.01	0.0	0.61063	0.62336	2.46426	2.47063

Table 4: Case 4



(a) $L=1$, $F=0.01$ (b) $L=2$, $F=0.01$

(c) $L=3$, $F=0.01$ (d) $L=4$, $F=0.01$

Figure 11: Case 4, F=0.01, L=1,2, 3, 4.

Remark 4.3. *For the splitting case, we get the non-zero case between two eigenvalues of the Stark operator, except for the ground state, see table 4. Moreover, to get a significant figure satisfying the boundary conditions, we used a numerical precision up to* 10^{-8}*. Indeed, if we used a less precisions some of the geometrical behaviors of eigenfunctions are in general not representative, see figure 11.*

5 Concluding remarks

In this work, we presented an analytical and computational study of Stark operators and precisely the self-adjoint operators on finite domains. We numerically analyzed interesting boundary conditions. Even, we used a lot of approximations, the presented computational result confirm and accurate all analytical ones. The splitting phenomena developed in this work indicates a perfect start to develop other similar physical result, namely in the proper Stark effect. We intend to study more realistic model by considering random behavior of electric fields.

6 Data availability statement

H. NAJAR : Sections 1,2,3 and 5.
M. Zahari: Section 4.

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