

Quantum cavities with alternating boundary conditions

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Abstract

We consider the quantum dynamics of a free nonrelativistic particle moving in a cavity and we analyze the effect of a rapid switching between two different boundary conditions. We show that this procedure induces, in the limit of infinitely frequent switchings, a new effective dynamics in the cavity related to a novel boundary condition. We obtain a dynamical composition law for boundary conditions which gives the emerging boundary condition in terms of the two initial ones.

Keywords: quantum boundary conditions, Trotter product formula, quadratic forms

(Some figures may appear in colour only in the online journal)

1. Introduction

Boundary conditions emerge as an effective description of the interaction between confined physical systems and their environment. In quantum theory, observables in physical systems are associated with self-adjoint operators [1]. In some cases, physical reasoning gives a formal expression for the Hamiltonian operator on a given Hilbert space. Such an operator is in general unbounded and, for this reason, it is necessary to consider the domain where it is defined.

Usually, one starts by considering some natural domain, where the operator is symmetric, and tries to verify whether the operator is self-adjoint or not. In the negative case one is forced to study various (if any) self-adjoint extensions of the operator under examination. Moreover, in the spirit of Stone's theorem [2], self-adjoint operators can be interpreted as the generators of the physical (unitary) transformations on the Hilbert space of physical states, so that, the choice

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of the ‘right’ self-adjoint extension is usually guided by physical intuition. For example, a free quantum particle confined in an impenetrable box is usually described in terms of the Laplace operator with Dirichlet boundary conditions. In this case it is necessary to impose the vanishing of the wave function at the boundary of the box in order to secure the unitarity of the dynamics.

Many authors have studied the connection between self-adjoint extensions and boundary conditions, see for example [3–8], and the latter have been proved to be useful in the descriptions of quantum phenomena in different areas of physics, ranging from atoms in cavities [9], to edge states in the quantum Hall effect [10], to quantum gravity and string theory [11].

Moreover, it is well known that the introduction of boundaries in quantum systems gives rise to peculiar phenomena like the Casimir effect. In its dynamical counterpart, photons can be generated in a microwave cavity as long as time-dependent boundary conditions are implemented [12].

Time-dependent boundary conditions [13, 14] can also produce a non-trivial Berry phase, as shown in [15]. Interestingly the simplest model of hyperbolic geometry, the Poincaré half-plane, emerges, bringing to light an unexpected link between geometry and quantum boundary conditions.

In this paper we will consider one of the paradigmatic examples of nonrelativistic quantum mechanics, that is, the case of a free particle confined in a cavity, i.e. in a region Ω of the n -dimensional space \mathbb{R}^n . The cavity is going to be subjected to a rapid switching between two different boundary conditions. We are going to show that the emerging dynamics, in the limit of infinitely frequent switchings, yields new boundary conditions obtained by suitably combining the initial ones.

This work represents the multidimensional generalization of the results in [16], where the 1D case, i.e. a free particle confined on an interval, is studied. The crucial difference between the 1D and the higher-dimensional case is the dimension of the boundary. If the particle is confined in a region $\Omega \subset \mathbb{R}^n$, the boundary $\partial\Omega$ is a manifold of dimension $n - 1$. Thus, if $n = 1$ and Ω is an interval its boundary has dimension zero and consists of two points. This means that there are only two boundary values for the wave function and other two for its derivative. In the n -dimensional case, with $n > 1$, the boundary values of a wave function are functions defined on $\partial\Omega$ and this aspect makes the extension to the general case very delicate. Indeed, for $n > 1$ the Hilbert space on the boundary is infinite dimensional, at variance with a finite-dimensional Hilbert space for $n = 1$. This entails the emergence of qualitatively new and interesting phenomena, which were not present in the 1D case.

The article is organized as follows. In section 2 we introduce the problem of composition law for boundary conditions and, after a short review of standard results about product formulas, we present our main result. In section 3, we revise the composition law for 1D systems, discussed in [16], in terms of a different approach, which will turn out to be suitable for the extension to the n -dimensional case. Finally, in section 4 some results on self-adjoint extensions are recalled and used for obtaining the composition law for a particle confined in an n -dimensional cavity with alternating boundary conditions. We finally draw our conclusions in section 5. In two appendices we also provide some technical results which turn out to be useful in section 4 to define the boundary data of a wave function in the n -dimensional case.

2. Trotter formula for alternating boundary conditions

Let us consider a quantum particle confined in a cavity $\Omega \subset \mathbb{R}^n$, where Ω is an open connected bounded set, whose boundary $\partial\Omega$ is a smooth submanifold of \mathbb{R}^n . We suppose that the particle is spinless, free and has a mass m . The description of this system is provided by the free Hamiltonian

$$T = \frac{p^2}{2m} = -\frac{1}{2m}\Delta, \tag{1}$$

that is the the kinetic energy operator (here and henceforth, Planck’s constant $\hbar = 1$). Here Δ is the Laplacian defined on some dense subspace of $L^2(\Omega)$, the Hilbert space of square integrable functions on Ω .

We are going to denote by \mathcal{H}_b the Hilbert space of the boundary values of all possible wave functions, which will be specified later. It can happen that the boundary value of a function in $L^2(\Omega)$ is a distribution (see the example at the end of appendix A). For this reason, as we are going to discuss later on, \mathcal{H}_b cannot be identified with the space of square integrable functions on the boundary, $L^2(\partial\Omega)$.

It was proved in [7, 8], that every unitary operator U acting on \mathcal{H}_b uniquely determines a well-defined physical realization of T , i.e a self-adjoint extension of T , denoted by T_U , identifying some boundary conditions. The relation between the self-adjoint extension T_U and the unitary operator U will be recalled in sections 3 and 4.

Now, consider T_{U_1} and T_{U_2} , two realizations of T , corresponding to two boundary conditions, given by U_1 and U_2 , unitary operators on \mathcal{H}_b . Moreover we let the two boundary conditions rapidly alternate.

More precisely, if the boundary conditions are switched at a rate t/N , the overall unitary evolution reads

$$\underbrace{\left(e^{-itT_{U_1}/N} e^{-itT_{U_2}/N} \right) \left(e^{-itT_{U_1}/N} e^{-itT_{U_2}/N} \right) \dots \left(e^{-itT_{U_1}/N} e^{-itT_{U_2}/N} \right)}_{N \text{ times}} \tag{2}$$

$$= \left(e^{-itT_{U_1}/N} e^{-itT_{U_2}/N} \right)^N.$$

Equation (2) is an example of Trotter’s product formula [17]. Similar evolutions show up in different contexts of quantum mechanics, for example, in the emerging dynamics associated with the quantum Zeno effect [18–21], as well as in remarkable applications in quantum chaos [22, 23]. Lastly, but not less importantly, the Trotter product formula is fundamental in a rigorous definition of Feynman’s path integral [24].

As already discussed in [16], the relevant question is to show whether in the $N \rightarrow +\infty$ limit—when the time interval between the switches goes to zero, the number of switches goes to infinite, while the total time $2t$ is kept constant—the evolution is given by

$$\left(e^{-itT_{U_1}/N} e^{-itT_{U_2}/N} \right)^N \rightarrow e^{-i2tT_W}, \quad N \rightarrow +\infty \tag{3}$$

in terms of a new realization of T , say T_W , associated with some boundary conditions specified by the boundary unitary W .

The answer to the limiting dynamics problem dates back to deep mathematical results on product formulas. Trotter [17] proved that for every A and B self-adjoint operators such that their sum is self-adjoint [on the intersection of their domains $D(A) \cap D(B)$] one gets

$$\left(e^{-itA/N} e^{-itB/N} \right)^N \rightarrow e^{-it(A+B)}, \quad N \rightarrow +\infty. \tag{4}$$

Unfortunately, the intersection of the domains of two self-adjoint extensions of T is too small, and $T_{U_1} + T_{U_2}$ is not self-adjoint (not even its closure!), so that this result cannot be applied to our case.

To overcome this obstruction it is sufficient to consider the quadratic forms associated with the operators (i.e. their expectation values), instead of the operators themselves. The expectation value of the kinetic energy in the state ψ is given by

$$t_U(\psi) = \langle \psi | T_U \psi \rangle_{L^2(\Omega)} = -\frac{1}{2m} \int_{\Omega} \overline{\psi(x)} \Delta \psi(x) dx. \quad (5)$$

From the mathematical point of view, t_U is the quadratic form associated with T_U , whose domain, as discussed in section 4.3, can be considerably larger than $D(T_U)$.

Starting from the kinetic energies t_{U_1} and t_{U_2} , one can build the quadratic form $t_{U_1} + t_{U_2}$ defined on the (dense) intersection $D = D(t_{U_1}) \cap D(t_{U_2})$. It can be proved [25] that if the sum of the forms is bounded from below there is one and only one self-adjoint operator denoted by $T_{U_1} \dot{+} T_{U_2}$, called the form sum operator of T_{U_1} and T_{U_2} , corresponding to the form $t_{U_1} + t_{U_2}$, i.e. such that

$$t_{T_{U_1} \dot{+} T_{U_2}} = t_{T_{U_1}} + t_{T_{U_2}}. \quad (6)$$

This idea, introduced by Kato [26], was elaborated by Lapidus [27] who found the ultimate version of the Trotter product formula:

$$\left(e^{-it_{U_1}/N} e^{-it_{U_2}/N} \right)^N \rightarrow e^{-it(T_{U_1} \dot{+} T_{U_2})}, \quad N \rightarrow +\infty, \quad (7)$$

when T_{U_1} and T_{U_2} are bounded from below. As a technical remark notice that, as a consequence of the weakening of the hypotheses, the convergence of the product formula when the operator sum is not self-adjoint is in a weaker topology than in Trotter's case; more precisely equation (4) holds pointwise in t , while its weaker counterpart (7) is valid only on average on t [28]. The validity of the above formula in a stronger topology is still a matter of investigation, as pointed out in [27, 28].

Summarizing, we have that

$$\lim_{N \rightarrow +\infty} \left(e^{-it_{U_1}/N} e^{-it_{U_2}/N} \right)^N = e^{-i2tT_W}, \quad (8)$$

where

$$T_W = \frac{T_{U_1} \dot{+} T_{U_2}}{2}. \quad (9)$$

Moreover T_W is a new realization of the operator T with new boundary conditions specified by a unitary operator W obtained combining U_1 and U_2 in a suitable way. The operator W is given by the composition law

$$W = U_1 \star U_2 := P_W + \mathcal{C} \left(\frac{\mathcal{C}^{-1}(V_{U_1})Q_{U_1} + \mathcal{C}^{-1}(V_{U_2})Q_{U_2}}{2} \right) Q_W, \quad (10)$$

where:

- U_i ($i = 1, 2$) can be uniquely decomposed into the sum $P_{U_i} + V_{U_i}$, where P_{U_i} is the spectral projection of U_i on the eigenspace with eigenvalue 1, $Q_{U_i} = I - P_{U_i}$, and $V_{U_i} = Q_{U_i} U_i Q_{U_i}$ is the restriction of U_i to the range of Q_{U_i} ;
- $Q_W = Q_{U_1} \wedge Q_{U_2}$ is the projection onto the intersection of the ranges of Q_{U_1} and Q_{U_2} , and $P_W = I - Q_W$ is the spectral projection of W onto its eigenspace with eigenvalue 1;
- the symbols \mathcal{C} and \mathcal{C}^{-1} denote, respectively, the Cayley transform and its inverse. As a matter of fact the Cayley transform maps the set of self-adjoint operators onto the set

of unitary operators which do not have 1 as an eigenvalue. In fact, for every self-adjoint operator A on a Hilbert space, the operator

$$\mathcal{C}(A) = (A - iI)(A + iI)^{-1}, \tag{11}$$

is unitary. Conversely, for every unitary operator V such that $I - V$ is invertible, the operator

$$\mathcal{C}^{-1}(V) = i(I + V)(I - V)^{-1}, \tag{12}$$

is self-adjoint on the range of $(I - V)$.

3. Composition law of boundary conditions for a free particle in a one-dimensional cavity

Before delving into the study of the composition law for boundary conditions in $\Omega \subset \mathbb{R}^n$, we would like to express the 1D results discussed in [16] in a different form, suitable for a generalization to higher dimensions.

Consider a free particle confined in the interval $\Omega = (0, 1)$. Its Hamiltonian is the 1D Laplacian,

$$T = \frac{p^2}{2m} = -\frac{1}{2m} \frac{d^2}{dx^2}, \tag{13}$$

acting on some dense subspace of $L^2(0, 1)$. Notice that in this 1D case, the boundary $\partial\Omega = \{0, 1\}$ consists of two points only and the Hilbert space of the boundary values is two dimensional, that is $\mathcal{H}_b = L^2(\{0, 1\}) = \mathbb{C}^2$.

As proved in [7], the whole family of self-adjoint extensions of T is in one-to-one correspondence with the possible boundary conditions coming out from $U(2)$, the set of 2×2 unitary matrices. More precisely, to each unitary $U \in U(2)$ there corresponds a unique self-adjoint extension

$$T_U = -\frac{1}{2m} \frac{d^2}{dx^2}, \tag{14}$$

acting on the domain

$$D(T_U) = \{\psi \in H^2(0, 1) : i(I + U)\varphi = (I - U)\dot{\varphi}\}, \tag{15}$$

where φ and $\dot{\varphi}$ are the boundary data of the wave function ψ and are defined by

$$\varphi = \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix}, \quad \dot{\varphi} = \begin{pmatrix} -\psi'(0) \\ \psi'(1) \end{pmatrix}. \tag{16}$$

We recall that $H^2(0, 1)$ is the Sobolev space of square integrable functions ψ with square integrable first and second derivative, respectively ψ' and ψ'' . Moreover any wave function ψ in the domain of T_U satisfies the boundary conditions

$$i(I + U)\varphi = (I - U)\dot{\varphi}. \tag{17}$$

Notice that this parametrization of the self-adjoint extensions of T in terms of boundary unitaries differs slightly from the one presented in [16]; nevertheless, the two parametrizations are equivalent.

Now consider the eigenprojection of U with eigenvalue 1, from now on denoted by P_U . Its orthogonal projection will be denoted by Q_U , such that $Q_U + P_U = I$. Notice that P_U can degenerate into the identity when $U = I$, as well as it can be the zero operator when 1 is not an eigenvalue of U .

By means of P_U and Q_U we are able to recast U in (17) into a sum on orthogonal eigenspaces, that is,

$$U = P_U + V_U, \quad V_U = UQ_U = Q_U U = Q_U U Q_U. \quad (18)$$

Notice that the operator V_U is unitary on the range of Q_U and 1 does not belong to its spectrum. Having this decomposition at hand, we can give an equivalent characterization of the domain of T_U by projecting equation (17) onto the ranges of P_U and Q_U :

$$i(I + U)\varphi = (I - U)\dot{\varphi} \iff \begin{cases} P_U \varphi = 0, \\ Q_U \dot{\varphi} = -K_U \varphi, \end{cases} \quad (19)$$

where K_U is (minus) the inverse Cayley transform of V_U , that is

$$K_U = -\mathcal{C}^{-1}(V_U)Q_U = -i(I + V_U)(I - V_U)^{-1}Q_U, \quad (20)$$

and $(I - V_U)^{-1}$ makes perfectly sense, since 1 is not an eigenvalue of V_U .

Equation (19) is valid for every unitary U , and particularizes to special forms according to the form of the spectral projection P_U . We can distinguish among three cases:

- (a) 1 is a double degenerate eigenvalue of U , therefore $P_U = I$. This corresponds to Dirichlet boundary conditions;
- (b) 1 is a nondegenerate eigenvalue of U , therefore $U = P_U + \lambda Q_U$, with $|\lambda| = 1$ and $\lambda \neq 1$. This case corresponds to: $Q_U \dot{\varphi} = i(1 + \lambda)(1 - \lambda)^{-1} Q_U \varphi$, $P_U \varphi = 0$;
- (c) 1 is not an eigenvalue of U , therefore $P_U = 0$. For example if $U = -I$, we find Neumann boundary conditions, which are a particular case of Robin boundary conditions. The latter correspond to

$$U = \begin{pmatrix} -e^{i\alpha_1} & 0 \\ 0 & -e^{i\alpha_2} \end{pmatrix}, \quad (21)$$

with $\alpha_1, \alpha_2 \in (-\pi, \pi)$, and

$$\psi'(0) = \tan \frac{\alpha_1}{2} \psi(0), \quad \psi'(1) = -\tan \frac{\alpha_2}{2} \psi(1). \quad (22)$$

Summing up: case (a) happens when $U = I$, which corresponds to a constraint on both the values of the wave function at the boundary. Case (b) provides, instead, one constraint on the values of the wave function at the boundary. For example, when $U = P_U - e^{i\alpha} Q_U$, with $\alpha \in (-\pi, \pi)$ and P_U being the projection onto the span of $(1, 0)$, we obtain

$$\psi(0) = 0 \quad \psi'(1) = -\tan \frac{\alpha}{2} \psi(1). \quad (23)$$

Finally, when 1 is not an eigenvalue, no constraint on the values of the wave function at the boundary arises from case (c). It is clear now how the behavior of the wave function at the boundary is related to the presence or the absence of the eigenvalue 1 of U .

3.1. Quadratic forms

In this subsection we analyze the relation between a self-adjoint operator T_U and its associated quadratic form t_U . First of all we will explain how to get the form t_U from the operator T_U and then we will show how to go in the opposite way.

Let T_U be a self-adjoint extension related to the unitary matrix $U \in U(2)$. An integration by parts yields

$$\begin{aligned} t_U(\psi) &= \langle \psi | T_U \psi \rangle_{L^2(0,1)} = -\frac{1}{2m} \int_0^1 \overline{\psi(x)} \psi''(x) \, dx \\ &= \frac{1}{2m} \left(\int_0^1 |\psi'(x)|^2 \, dx - \overline{\psi(1)} \psi'(1) + \overline{\psi(0)} \psi'(0) \right) \\ &= \frac{1}{2m} \left(\|\psi'\|_{L^2(0,1)}^2 - \langle \varphi | \dot{\varphi} \rangle_{\mathbb{C}^2} \right), \quad \text{for all } \psi \in D(T_U), \end{aligned}$$

where φ and $\dot{\varphi}$ are the boundary data (16), and $\langle \alpha | \beta \rangle_{\mathbb{C}^2} = \bar{\alpha}_1 \beta_1 + \bar{\alpha}_2 \beta_2$ is the canonical scalar product in \mathbb{C}^2 . Therefore, the expectation value of the kinetic energy of the particle has both contributions from the bulk and from the boundary. Making use of the boundary conditions given by equation (19), we can express the boundary contribution in a more convenient form by trading the boundary values of the derivative for the boundary values of the function. Indeed, one gets

$$\langle \varphi | \dot{\varphi} \rangle_{\mathbb{C}^2} = \langle (P_U + Q_U) \varphi | \dot{\varphi} \rangle_{\mathbb{C}^2} = \langle \varphi | Q_U \dot{\varphi} \rangle_{\mathbb{C}^2} = -\langle \varphi | K_U \varphi \rangle_{\mathbb{C}^2}, \quad (24)$$

whence

$$t_U(\psi) = \frac{1}{2m} \left(\|\psi'\|_{L^2(0,1)}^2 + \langle \varphi | K_U \varphi \rangle_{\mathbb{C}^2} \right), \quad \text{for all } \psi \in D(T_U). \quad (25)$$

Therefore, since $D(T_U)$ is a core of t_U , the form domain $D(t_U)$ is given by

$$D(t_U) = \{ \psi \in H^1(0,1) : P_U \varphi = 0 \}, \quad (26)$$

where, $H^1(0,1)$ is the Sobolev space of square integrable functions with square integrable first derivative.

The quadratic form t_U is closed and bounded from below, that is:

$$t_U(\psi) \geq -C \|\psi\|_{L^2(0,1)}^2, \quad \text{for all } \psi \in D(t_U), \quad (27)$$

for some constant C depending on the norm $\|K_U\|$ and on the continuity of the restriction map

$$\psi \in H^1(0,1) \mapsto \varphi = \psi|_{\partial\Omega} = \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix} \in \mathbb{C}^2. \quad (28)$$

Therefore the quadratic form t_U associated with a generic self-adjoint extension T_U of T has the following properties:

- the value of the form (25) at the wave function ψ is given by the sum of two terms: the first one is common to all the extensions while the second one depends explicitly on the extension. Notice, indeed, that the matrix K_U in (20) is, up to a sign, the inverse Cayley transform of the unitary matrix U with its eigenvalue 1 stripped out;
- the form domain $D(t_U)$ in (26) is expressed in terms of P_U , the eigenprojection of U with eigenvalue 1;
- the form t_U is closed and bounded from below and its lower bound in (27) depends on the norm of the self-adjoint matrix K_U and on the continuity of the restriction map (28).

Next, we are going to explain how to obtain the self-adjoint operator from the quadratic form. We consider a quadratic form t having the same properties explained above, namely such that

$$t(\psi) = \frac{1}{2m} \left(\|\psi'\|_{L^2(0,1)}^2 + \langle \varphi | K \varphi \rangle_{\mathbb{C}^2} \right), \quad D(t) = \{\psi \in H^1(0,1) : P\varphi = 0\}, \quad (29)$$

where $K = K^\dagger$ is a self-adjoint matrix and P an orthogonal projection, such that $KP = PK = 0$.

As above, one can show that the form t is closed and bounded from below. There is a one-to-one correspondence between the set of closed and bounded from below quadratic forms and the set of bounded from below self-adjoint operators [25], known as representation theorem. Using this correspondence one can immediately recover the self-adjoint extension T_U associated with the form t :

$$D(T_U) = \{\psi \in H^2(0,1) : i(I+U)\varphi = (I-U)\dot{\varphi}\} \quad (30)$$

where the unitary matrix U is given by

$$U = P - \mathcal{C}(K)Q. \quad (31)$$

$Q = I - P$, and \mathcal{C} is the Cayley transform defined in (11). Notice that P is the eigenprojection of U with eigenvalue 1 and that Q is its orthogonal projection.

3.2. Composition law of boundary conditions

We now evaluate the limit of the alternating dynamics (3). As already discussed, the product formula (3) holds with the form sum $T_W = \frac{1}{2}(T_{U_1} \dot{+} T_{U_2})$. Thus, the evaluation of the emergent dynamics in (3) requires the computation of the sum

$$t_{12}(\psi) = \frac{t_{U_1}(\psi) + t_{U_2}(\psi)}{2} = \frac{1}{2m} \left(\|\psi'\|_{L^2(0,1)}^2 + \langle \varphi | K_{12} \varphi \rangle_{\mathbb{C}^2} \right), \quad (32)$$

$$K_{12} = \frac{1}{2}(K_{U_1} + K_{U_2}),$$

where the form domain reads

$$D(t_{12}) = D(t_{U_1}) \cap D(t_{U_2}) = \{\psi \in H^1(0,1) : P_{U_1}\varphi = 0 = P_{U_2}\varphi\}. \quad (33)$$

Notice that K_{12} is a self-adjoint matrix, since both K_{U_1} and K_{U_2} are. Let $Q_{12} = Q_{U_1} \wedge Q_{U_2}$ be the orthogonal projection onto the intersection of the ranges of Q_{U_1} and Q_{U_2} , that is

$$\text{Ran}(Q_{12}) = \text{Ran}(Q_{U_1}) \cap \text{Ran}(Q_{U_2}). \quad (34)$$

Moreover define

$$P_{12} = I - Q_{12}. \quad (35)$$

Then, the form domain of t_{12} can be written in terms of the orthogonal projection P_{12} as

$$D(t_{12}) = \{\psi \in H^1(0,1) : P_{12}\varphi = 0\} \quad (36)$$

since the kernel of P_{12} is given by

$$N(P_{12}) = \text{Ran}(Q_{12}) = N(P_{U_1}) \cap N(P_{U_2}). \quad (37)$$

Since t_{12} is closed and bounded from below by the representation theorem [25], there is a unique (bounded from below) self-adjoint operator T_W such that

$$\begin{aligned} D(T_W) &= \{\psi \in H^2(0, 1) : i(I + W)\varphi = (I - W)\dot{\varphi}\}, \\ t_{12}(\psi) &= \langle \psi | T_W \psi \rangle \quad \text{for all } \psi \in D(T_W). \end{aligned} \tag{38}$$

Here the unitary matrix $W \in U(2)$ is given by

$$W = P_{12} - \mathcal{C}(K_{12})Q_{12}, \tag{39}$$

and $\mathcal{C}(K_{12})$ is the Cayley transform of K_{12} on the range of Q_{12} . Since P_{12} is the eigenprojection of W with eigenvalue 1, in accordance with our convention we have that $P_{12} = P_W$, $Q_{12} = Q_W$ and $K_{12} = K_W$. Notice that

$$K_{U_i} = -\mathcal{C}^{-1}(V_{U_i})Q_{U_i}, \quad i = 1, 2, \tag{40}$$

thus we obtain that (39) is exactly the formula (10) in the 1D case.

3.3. The path to higher dimensions

Here we first sum up the main steps of the construction of the composition law of boundary conditions in the 1D case, i.e. $\Omega = (0, 1)$, and then we introduce the main ideas to extend the result to the general n -dimensional case.

- (i) First of all we have introduced the Hilbert space of boundary values $\mathcal{H}_b = \mathbb{C}^2$, then we have defined the boundary data of a wave function

$$\psi \in H^2(0, 1) \mapsto (\varphi, \dot{\varphi}) \in \mathcal{H}_b \times \mathcal{H}_b, \tag{41}$$

with φ and $\dot{\varphi}$ being given by (16), and finally we have recalled the one-to-one correspondence (15) between unitary operators acting on \mathcal{H}_b and the self-adjoint extensions of T .

- (ii) We have shown that the quadratic form (25) associated with each self-adjoint extension of T is given by the sum of two terms, the first one being independent of the extension and the second one depending on the extension through the self-adjoint matrix $K_U = -\mathcal{C}^{-1}(V_U)Q_U$. The form domain $D(t_U)$ in (26) is expressed in terms of the eigenprojection P_U with eigenvalue 1 of the unitary matrix U specifying the extension. Moreover the form t_U is closed and bounded from below and its lower bound depends on the norm of K_U and the continuity of the restriction map (28).

Conversely, given a quadratic form t (29), with P being an orthogonal projection and K a self-adjoint matrix, with $PK = KP = 0$, we have seen how to obtain the boundary unitary matrix U by (31).

- (iii) Finally we have considered two different self-adjoint extensions of T , say T_{U_1} and T_{U_2} , with $U_1, U_2 \in U(2)$, and we have evaluated the limit of the alternating dynamics (3). We have studied the sum of the quadratic forms (32), on the domain (36), where P_{12} is the orthogonal projection whose kernel is the intersection of the kernels of P_{U_1} and P_{U_2} . Therefore, the unique self-adjoint operator T_W associated with t_{12} is specified by the unitary matrix W obtained by a composition of U_1 and U_2 :

$$W = U_1 * U_2 = P_{12} - \mathcal{C}(K_{12})Q_{12} \tag{42}$$

with $Q_{12} = I - P_{12}$.

Now we retrace this procedure and we explain step by step the strategy to extend it to n dimensions, i.e. to $\Omega \subset \mathbb{R}^n$.

- The first difficulty is the definition of the boundary data

$$\psi \in L^2(\Omega) \mapsto (\varphi, \dot{\varphi}) \in \mathcal{H}_b \times \mathcal{H}_b, \quad (43)$$

and the identification of the Hilbert space of boundary values \mathcal{H}_b . Once these aspects are clarified, the one-to-one correspondence between the unitary operators acting on \mathcal{H}_b and the self-adjoint extensions of the operator T will hold as well as in the 1D case. See [8].

- Given $U \in \mathbf{U}(\mathcal{H}_b)$ we will study the quadratic form t_U associated with T_U . Mimicking the 1D case we will find that t_U is given by

$$t_U(\psi) = \frac{1}{2m} \left(\|\nabla \psi_D\|_{L^2(\Omega)}^2 + \langle \varphi | K_U \varphi \rangle_{\mathcal{H}_b} \right), \quad (44)$$

where ψ_D is the ‘regular component’ of ψ , which vanishes at the boundary, while K_U is a self-adjoint operator defined by

$$K_U = -\mathcal{C}^{-1}(V_U)Q_U, \quad Q_U = I - P_U, \quad V_U = Q_U U Q_U, \quad (45)$$

and P_U is the eigenprojection of U with eigenvalue 1. Understanding the meaning of ψ_D is one of the main difficulties in the study of the quadratic form t_U . A further complication arises from the fact that, in the n -dimensional case, the operator K_U can be unbounded. This means that the form t_U is not, in general, bounded from below. In order to avoid this problem, we will consider only unitary operators $U \in \mathbf{U}(\mathcal{H}_b)$ having a spectrum with a gap around the point 1: this condition ensures that K_U is bounded.

- Finally, we will extend the composition law for boundary conditions assuming that the spectra of $U_1, U_2 \in \mathbf{U}(\mathcal{H}_b)$ are both gapped around the point 1. This compatibility condition is necessary to extend the construction of the composition $U_1 * U_2$ to the n -dimensional case because it ensures that the form sum t_{12} is densely defined, closed and bounded from below, and allows us to identify the self-adjoint extension corresponding to t_{12} .

4. A composition law for a free particle in a cavity

In this section we are going to extend the composition law determined in section 3.2. Since we are going to describe a free particle in a cavity Ω we need some results about self-adjoint extensions of the operator T in terms of boundary conditions. This was largely discussed in [7, 8].

4.1. The framework

Let Ω be an open bounded set in \mathbb{R}^n , whose boundary is regular. Let ν be the normal to $\partial\Omega$, by convention ν is oriented towards the exterior of Ω . We define for a regular function ψ its normal derivative along ν :

$$\partial_\nu \psi = \nu \cdot (\nabla \psi) |_{\partial\Omega}. \quad (46)$$

Notice that, by definition, $\partial_\nu \psi$ is a function settled on $\partial\Omega$.

We consider the operator

$$T = -\frac{1}{2m} \Delta, \quad (47)$$

defined on some dense subset of $L^2(\Omega)$, for example $\mathcal{D}(\Omega)$, the space of test functions in Ω (compactly supported and smooth functions in Ω). Wave functions on this space are not able

to provide information about the boundary because for every $\psi \in \mathcal{D}(\Omega)$: $\psi|_{\partial\Omega} = \partial_\nu\psi = 0$. Let T^\dagger be the adjoint of T with domain

$$D(T^\dagger) = \{\psi \in L^2(\Omega) : \Delta\psi \in L^2(\Omega)\}. \quad (48)$$

We are going to identify the Hilbert space of the boundary values \mathcal{H}_b . It can be proved [29] that the ‘restriction’ to the boundary $\partial\Omega$ of a wave function $\psi \in D(T^\dagger)$, denoted by $\psi|_{\partial\Omega}$, belongs to $H^{-\frac{1}{2}}(\partial\Omega)$, the fractional Sobolev space of order $-1/2$. Therefore in the n -dimensional case the Hilbert space of boundary values $\mathcal{H}_b = H^{-\frac{1}{2}}(\partial\Omega)$ is infinite dimensional, unlike the 1D case.

We are now ready to state the following result, proved in [8], about the self-adjoint extensions of T .

Theorem 4.1. *The set of all self-adjoint extensions of T is*

$$\{T_U : D(T_U) \rightarrow L^2(\Omega), U \in \mathbf{U}(\mathcal{H}_b)\}, \quad (49)$$

where for all $U \in \mathbf{U}(\mathcal{H}_b)$

$$D(T_U) = \{\psi \in D(T^\dagger) : i(I + U)\varphi = (I - U)\dot{\varphi}\}, \quad (50)$$

and the boundary data $(\varphi, \dot{\varphi})$ are specified in equation (54).

In the 1D case, equation (17) provided a thorough parametrization of the self-adjoint extensions of the operator T . Theorem 4.1 states that equation (17) is still valid for a general $\Omega \subset \mathbb{R}^n$ through a suitable identification of the boundary data $(\varphi, \dot{\varphi})$. In what follows we would like to provide the reader with explanations about the boundary data $(\varphi, \dot{\varphi})$.

As discussed above, the restriction $\psi|_{\partial\Omega}$ of a wave function $\psi \in D(T^\dagger)$ to the boundary $\partial\Omega$ belongs to $\mathcal{H}_b = H^{-\frac{1}{2}}(\partial\Omega)$, while its normal derivative $\partial_\nu\psi$ belongs to a more irregular space (more precisely $\partial_\nu\psi$ belongs to $H^{-\frac{3}{2}}(\partial\Omega)$) [29].

For this reason equation (17) cannot hold by naively interpreting the boundary data $(\varphi, \dot{\varphi})$ as the pair $(\psi|_{\partial\Omega}, \partial_\nu\psi)$. Indeed, the elements of the pair are settled on different Hilbert spaces and the existence of an operator U acting both on $\psi|_{\partial\Omega}$ and $\partial_\nu\psi$ becomes meaningless. Moreover, the boundary values $\psi|_{\partial\Omega}$ and $\partial_\nu\psi$ are *not* independent data, as discussed in appendix A, and one can show that only the normal derivative of a ‘regular’ component ψ_D of ψ is independent of $\psi|_{\partial\Omega}$.

In order to define the regular component ψ_D of ψ , we need a useful decomposition of the domain of the adjoint $D(T^\dagger)$ given in (48):

$$D(T^\dagger) = D(T_D) + N(T^\dagger), \quad \psi = \psi_D + \psi_0, \quad (51)$$

where T_D is the self-adjoint extension of T with Dirichlet boundary conditions, that is on the domain

$$D(T_D) = \{\psi \in H^2(\Omega) : \psi|_{\partial\Omega} = 0\}, \quad (52)$$

and

$$N(T^\dagger) = \{\psi \in D(T^\dagger) : \Delta\psi = 0\} \quad (53)$$

is the kernel of T^\dagger . In other words, every $\psi \in D(T^\dagger)$ can be uniquely decomposed in the sum $\psi_D + \psi_0$, where $\psi_D \in D(T_D)$ is a function vanishing on the boundary, $\psi_D|_{\partial\Omega} = 0$, and ψ_0 is a harmonic function, $\Delta\psi_0 = 0$. See appendix A for more details.

We are finally in the right position to define the boundary data $(\varphi, \dot{\varphi})$ of a wave function $\psi \in D(T^\dagger)$:

$$\varphi = \psi|_{\partial\Omega} = \psi_0|_{\partial\Omega}, \quad \dot{\varphi} = \Lambda \partial_\nu \psi_D, \quad (54)$$

where ψ_D is the regular component of ψ in the sense of the decomposition (51). Here $\Lambda = (I - \Delta_{\partial\Omega})^{\frac{1}{2}}$, where $\Delta_{\partial\Omega}$ is the Laplace–Beltrami operator on $\partial\Omega$ [30], and its role is merely to pull back $\partial_\nu \psi_D \in H^{\frac{1}{2}}(\partial\Omega)$ to $\mathcal{H}_b = H^{-\frac{1}{2}}(\partial\Omega)$, the common Hilbert space of the boundary data. Any unitary map from $H^{\frac{1}{2}}(\partial\Omega)$ to $H^{-\frac{1}{2}}(\partial\Omega)$ will do, and the reader can safely ignore its presence henceforth.

For further mathematical details see [8].

4.2. Parametrization of the self-adjoint extensions of T by means of spectral projections

It is of interest to recast the former parametrization of T_U by isolating the contribution of the eigenvalue 1 from the spectrum of U and expressing it in terms of spectral projections.

In analogy with section 3 we define P_U as the eigenprojection of U with eigenvalue 1 and $Q_U = I - P_U$ its orthogonal projection.

Then, the unitary operator U can be decomposed in the sum $U = P_U + V_U$, where $V_U = Q_U U Q_U$. After projecting onto the two mutually orthogonal subspaces given by P_U and Q_U , the domain of T_U reads

$$D(T_U) = \{\psi \in D(T^\dagger) : P_U \varphi = 0, Q_U \dot{\varphi} = -K_U \varphi\}, \quad (55)$$

where K_U is given by (minus) the Cayley transform of V_U ,

$$K_U = -\mathcal{C}^{-1}(V_U)Q_U = -i(I + V_U)(I - V_U)^{-1}Q_U. \quad (56)$$

Even in higher dimensions the operator $(I - V_U)$ is invertible, since the eigenvalue 1 was stripped out, but it may be unbounded. The operator $(I - V_U)^{-1}$ will be bounded as long as 1 does not belong to the spectrum of V_U , that is as long as the spectrum of U has a gap around the point 1 (figure 1). For this reason, from now on, we are going to make the latter our working assumption [31].

4.3. Quadratic forms

As already sketched for the 1D case we provide an explicit expression for the expectation value of the kinetic energy of a free particle in a cavity Ω .

We are going to prove that the expectation value of the kinetic energy T_U is

$$t_U(\psi) = \frac{1}{2m} \left(\|\nabla \psi_D\|_{L^2(\Omega)}^2 + \langle \varphi | K_U \varphi \rangle_{\mathcal{H}_b} \right), \quad (57)$$

where ψ_D is the regular component of ψ in the sense of the decomposition (51), K_U is the operator defined in (56) and $\mathcal{H}_b = H^{-\frac{1}{2}}(\partial\Omega)$.

Take $\psi \in D(T_U) \cap C^\infty(\bar{\Omega})$, since $D(T_U) \subset D(T^\dagger) = D(T_D) + N(T^\dagger)$, it follows that it can be decomposed as $\psi = \psi_D + \psi_0$. Therefore,

$$\begin{aligned} 2m t_U(\psi) &= -\langle \psi | \Delta \psi \rangle_{L^2(\Omega)} = -\langle \psi | \Delta \psi_D \rangle_{L^2(\Omega)} - \langle \psi | \Delta \psi_0 \rangle_{L^2(\Omega)} \\ &= -\langle \psi | \Delta \psi_D \rangle_{L^2(\Omega)} = -\langle \psi_D | \Delta \psi_D \rangle_{L^2(\Omega)} - \langle \psi_0 | \Delta \psi_D \rangle_{L^2(\Omega)}, \end{aligned} \quad (58)$$

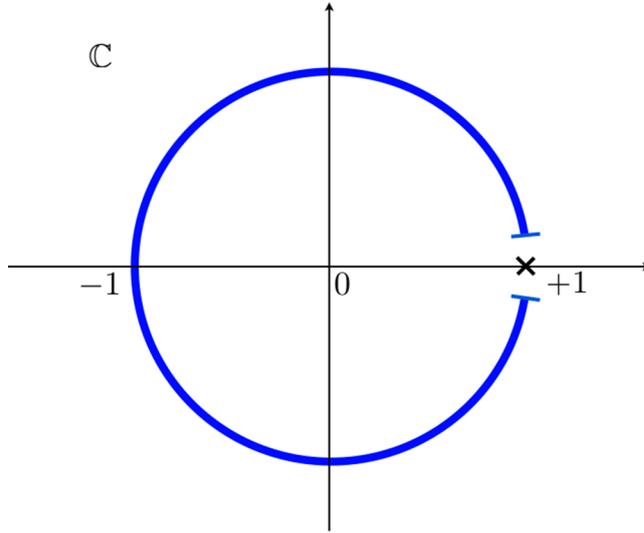


Figure 1. The spectrum of U has a gap around the point 1 in the complex plane.

where we used twice the decomposition of ψ and once the property $\Delta\psi_0 = 0$. Next by means of the Gauss-Green formulas we will show that

- (i) $\langle \psi_{\mathbb{D}} | \Delta\psi_{\mathbb{D}} \rangle_{L^2(\Omega)} = -\|\nabla\psi_{\mathbb{D}}\|_{L^2(\Omega)}^2$;
- (ii) $\langle \psi_0 | \Delta\psi_{\mathbb{D}} \rangle_{L^2(\Omega)} = \langle \psi | \partial_{\nu}\psi_{\mathbb{D}} \rangle_{L^2(\partial\Omega)}$;

so that, by putting them together, we obtain

$$2m t_U(\psi) = \|\nabla\psi_{\mathbb{D}}\|_{L^2(\Omega)}^2 - \langle \psi | \partial_{\nu}\psi_{\mathbb{D}} \rangle_{L^2(\partial\Omega)}. \tag{59}$$

Let us begin from (i):

$$\begin{aligned} \langle \psi_{\mathbb{D}} | \Delta\psi_{\mathbb{D}} \rangle_{L^2(\Omega)} &= \int_{\Omega} \overline{\psi_{\mathbb{D}}(x)} \Delta\psi_{\mathbb{D}}(x) \, dx = - \int_{\Omega} |\nabla\psi_{\mathbb{D}}(x)|^2 \, dx + \int_{\partial\Omega} \overline{\psi_{\mathbb{D}}} \partial_{\nu}\psi_{\mathbb{D}} \, dS \\ &= - \int_{\Omega} |\nabla\psi_{\mathbb{D}}(x)|^2 \, dx = -\|\nabla\psi_{\mathbb{D}}\|_{L^2(\Omega)}^2, \end{aligned} \tag{60}$$

where we used the property $\psi_{\mathbb{D}}|_{\partial\Omega} = 0$.

Next we move on to the computation of (ii). Notice first that

$$\int_{\Omega} \overline{\nabla\psi_{\mathbb{D}}(x)} \cdot \nabla\psi_0(x) \, dx = - \int_{\Omega} \overline{\psi_{\mathbb{D}}(x)} \Delta\psi_0(x) \, dx + \int_{\partial\Omega} \overline{\psi_{\mathbb{D}}} \partial_{\nu}\psi_0 \, dS = 0, \tag{61}$$

since $\psi_{\mathbb{D}}|_{\partial\Omega} = 0$ and $\Delta\psi_0 = 0$. Therefore,

$$\begin{aligned} \langle \psi_0 | \Delta\psi_{\mathbb{D}} \rangle_{L^2(\Omega)} &= \int_{\Omega} \overline{\psi_0(x)} \Delta\psi_{\mathbb{D}}(x) \, dx = - \int_{\Omega} \overline{\nabla\psi_0(x)} \cdot \nabla\psi_{\mathbb{D}}(x) \, dx + \int_{\partial\Omega} \overline{\psi_0} \partial_{\nu}\psi_{\mathbb{D}} \, dS \\ &= \int_{\partial\Omega} \overline{\psi} \partial_{\nu}\psi_{\mathbb{D}} \, dS = \langle \psi | \partial_{\nu}\psi_{\mathbb{D}} \rangle_{L^2(\partial\Omega)}, \end{aligned} \tag{62}$$

where we made use of equation (61) and the equality $\psi_0|_{\partial\Omega} = \psi|_{\partial\Omega}$.

Putting together all the ingredients we find that, for all $\psi \in D(T_U) \cap C^\infty(\overline{\Omega})$,

$$\begin{aligned} 2m t_U(\psi) &= \|\nabla \psi_D\|_{L^2(\Omega)}^2 - \langle \psi | \partial_\nu \psi_D \rangle_{L^2(\partial\Omega)} \\ &= \|\nabla \psi_D\|_{L^2(\Omega)}^2 - \langle \varphi | \dot{\varphi} \rangle_{\mathcal{H}_b} = \|\nabla \psi_D\|_{L^2(\Omega)}^2 + \langle \varphi | K_U \varphi \rangle_{\mathcal{H}_b}, \end{aligned} \quad (63)$$

where we used the definition of the boundary values $(\varphi, \dot{\varphi})$ in (54) and the boundary conditions in (55). By a density argument one finally gets (57) for all $\psi \in D(T_U)$.

The mathematical expression of the kinetic energy t_U of a free particle in a cavity Ω highly resembles the one given in equation (25) for the 1D case. Though this apparent similarity, the two equations differ considerably. For example the contribution from the bulk is due to the regular part of ψ , that is ψ_D , rather than from the whole function. Moreover the boundary term is in general unbounded. It is bounded as long as K_U is bounded, which is guaranteed by the condition of U with gapped spectrum.

Finally, since $D(T_U)$ is a core of t_U we find that

$$D(t_U) = \{\psi \in H_0^1(\Omega) + N(T^\dagger) : P_U \varphi = 0\}, \quad (64)$$

where $H_0^1(\Omega)$ is the subspace of $H^1(\Omega)$ whose functions vanish at the boundary. For more details see [8].

4.4. Composition law

We now evaluate the limit of the alternating dynamics (8) in the case of a free particle confined in a cavity $\Omega \subset \mathbb{R}^n$. Once more the product formula (8) holds with the form sum

$$T_W = \frac{T_{U_1} + T_{U_2}}{2}. \quad (65)$$

Following the 1D case we carry on the computation of the sum

$$\begin{aligned} t_{12}(\psi) &= \frac{t_{U_1}(\psi) + t_{U_2}(\psi)}{2} = \frac{1}{2m} \left(\|\nabla \psi_D\|_{L^2(\Omega)}^2 + \langle \varphi | K_{12} \varphi \rangle_{\mathcal{H}_b} \right), \\ K_{12} &= \frac{1}{2} (K_{U_1} + K_{U_2}), \end{aligned} \quad (66)$$

and its domain

$$D(t_{12}) = \{\psi \in H_0^1(\Omega) + N(T^\dagger) : P_{12} \varphi = 0\}. \quad (67)$$

We stress that K_{12} is a bounded self-adjoint operator, since both K_{U_1} and K_{U_2} are, and thus the quadratic form t_{12} is closed and bounded from below. Therefore, by the representation theorem [25], there exists a unique self-adjoint extension T_W of T such that

$$t_{12}(\psi) = \langle \psi | T_W \psi \rangle_{L(\Omega)}, \quad \text{for all } \psi \in D(T_W), \quad (68)$$

where

$$D(T_W) = \{\psi \in D(T^\dagger) : i(I + W)\varphi = (I - W)\dot{\varphi}\}. \quad (69)$$

We stress that $P_W = P_{12}$, so that W can be explicitly built from P_{12} and K_{12} as

$$W = P_{12} - \mathcal{C}(K_{12})Q_{12}, \quad (70)$$

where $\mathcal{C}(K_{12})$ is the Cayley transform of K_{12} on the range of Q_{12} . This complete our proof of equation (10).

For the sake of the mathematically oriented reader we finally gather our main result in the guise of a theorem:

Theorem 4.2. *Let Ω be an open bounded set in \mathbb{R}^n , whose boundary is regular. Consider two self-adjoint extensions T_{U_1} and T_{U_2} of the kinetic energy operator $T = -\frac{1}{2m}\Delta$, given by theorem 4.1, and assume that the boundary unitaries U_1 and U_2 are both gapped around the point 1. Then the operator $W = U_1 \star U_2$ given by the composition law (10) is unitary, and one has*

$$\lim_{N \rightarrow +\infty} \int_{\mathbb{R}} dt f(t) \left(e^{-itT_{U_1}/N} e^{-itT_{U_2}/N} \right)^N \psi = \int_{\mathbb{R}} dt f(t) e^{-i2tT_W} \psi, \quad (71)$$

for every compactly supported continuous function f and for every vector $\psi \in L^2(\Omega)$.

A final remark is in order. We recall that the gap condition (see figure 1) was crucial in ensuring that the self-adjoint boundary operators K_{U_1} and K_{U_2} defined in (56) are bounded, so that their sum is self-adjoint and thus W is unitary. However, such condition is not necessary at all and the hypotheses of theorem 4.2 can be relaxed. For example, by making use of more refined results of operator theory, one can extend the theorem to semi-gapped boundary unitaries (see figure B1). The interested reader can look at appendix B for more details.

5. Conclusions

We have studied the dynamics of a quantum particle confined in a cavity subject to two rapidly alternating boundary conditions. The limit dynamics has been expressed in terms of new boundary conditions, which have emerged from a dynamical composition law.

Differences and similarities between the 1D and the n -dimensional case have been shown and largely discussed. While in the 1D case the composition law is expressed in terms of unitary matrices, in the n -dimensional case, instead, it is obtained through unitary operators on an infinite dimensional Hilbert space. For this reason the spectral properties of the operators have to be taken into consideration and handled with care.

In the end, in the near future it would be interesting both to apply the aforementioned results to cavities having interesting geometrical properties, e.g. with nonregular boundaries [34], and to analyze the case of the Dirac operator [35].

Further investigations will involve concrete analysis and applications such as the Casimir effect or the quantum Hall effect.

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Appendix A. A useful decomposition

In this appendix we would like to provide the reader with further details about the decomposition of the domain (48),

$$D(T^\dagger) = D(T_D) + N(T^\dagger), \tag{A.1}$$

where

$$D(T_D) = \{\psi \in H^2(\Omega) : \psi|_{\partial\Omega} = 0\}, \quad N(T^\dagger) = \{\psi \in L^2(\Omega) : \Delta\psi = 0\}. \tag{A.2}$$

As explained in section 4, this decomposition is crucial to define the regularized normal derivative of a wave function and its boundary data $(\varphi, \dot{\varphi})$ in (54). Moreover, it enters in the definition of the kinetic energy (57).

In order to understand the meaning of this decomposition, we explain here how to decompose a smooth function $\psi \in C^\infty(\overline{\Omega}) \subset D(T^\dagger)$ into the sum $\psi = \psi_D + \psi_0$, with $\psi_D|_{\partial\Omega} = 0$ and $\Delta\psi_0 = 0$. First of all we define $g = \psi|_{\partial\Omega}$ and solve the (boundary value) electrostatic problem:

$$\begin{cases} -\Delta u = 0 & \text{on } \Omega \\ u = g & \text{in } \partial\Omega. \end{cases} \tag{A.3}$$

The solution ψ_0 of (A.3) represents the electrostatic potential in the cavity Ω with the given value $g = \psi|_{\partial\Omega}$ on the boundary. Next, we define ψ_D as $\psi - \psi_0$; manifestly $\psi_D|_{\partial\Omega} = 0$. Therefore we can write $\psi = \psi_D + \psi_0$ with $\psi_D|_{\partial\Omega} = 0$ and $\Delta\psi_0 = 0$. This decomposition can be extended by a density argument [32] to $D(T^\dagger)$, obtaining (A.1).

Notice that $D(T_D)$ represents the domain of a self-adjoint extension of T (the one specified by Dirichlet boundary conditions) and it is made up by much more regular functions than $N(T^\dagger)$. In fact, the space $N(T^\dagger)$ contains functions that can be very irregular on $\partial\Omega$. This is a fairly interesting phenomenon in potential theory: a harmonic function, which is extremely regular (analytic) in the interior of Ω can become very irregular on its boundary.

For example, consider the function $f(x, y) = 1/z = 1/(x + iy)$ in the upper half-plane $\Omega = \{(x, y) \in \mathbb{R}^2 : y > 0\}$. It is evident that though being harmonic on Ω , the function f diverges at the point $(0, 0) \in \partial\Omega$. In fact, its boundary value is a distribution! Indeed one gets

$$\lim_{y \downarrow 0} f(x, y) = P.V. \frac{1}{x} - i\pi\delta(x), \tag{A.4}$$

where $P.V.$ is the Cauchy principal value and δ the Dirac delta.

Appendix B. Semi-gapped boundary unitaries

In this appendix we consider the extension of the composition law (10) to boundary unitaries U_i which are not gapped, and thus to unbounded boundary operators K_{U_i} . In general the sum of two unbounded (self-adjoint) operators $K_{U_1} + K_{U_2}$ is a touchy business. However, if the two operators are bounded from below, the situation can be kept somewhat under control.

It can be proved [33] that a self-adjoint extension T_U of T is bounded from below as long as the corresponding operator K_U , which appears in equation (56), is bounded from below. In turn, by the properties of the Cayley transform (11), it is easy to see that K_U is bounded from below if and only the spectrum of U has a gap just below the point 1, namely the set $\{e^{i\alpha} : \alpha \in (-\varepsilon, 0)\}$ belongs to the resolvent set of U for some $\varepsilon > 0$. We will call such a U semi-gapped. See figure B1, where $\beta = -\cot(\varepsilon/2)$.

Suppose then that T_{U_1} and T_{U_2} are bounded below self-adjoint operators. We remind the reader that the hypothesis of boundedness from below is fundamental for the Trotter–Kato formula (7) to hold. Next, consider the sum of their quadratic forms

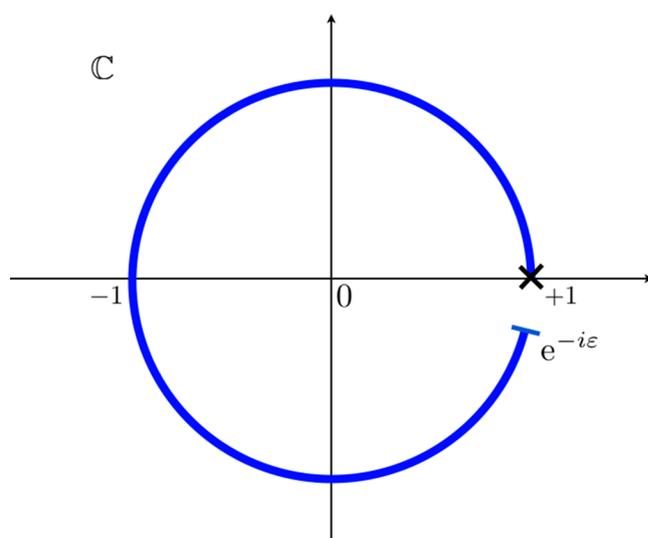


Figure B1. If K_U is bounded from below then the spectrum of V_U has a gap in the spectrum just below the point 1.

$$t_{12}(\psi) = \frac{t_{U_1}(\psi) + t_{U_2}(\psi)}{2} = \frac{1}{2m} \left(\|\nabla\psi_D\|_{L^2(\Omega)}^2 + \langle \varphi | K_{12}\varphi \rangle_{\mathcal{H}_b} \right),$$

$$K_{12} = \frac{1}{2} (K_{U_1} + K_{U_2}), \quad D(K_{12}) = D(K_1) \cap D(K_2). \tag{B.1}$$

It is defined on the domain

$$D(t_{12}) = D(t_{U_1}) \cap D(t_{U_2}) = \{ \psi \in H_0^1(\Omega) + N(T^\dagger) : P_{12}\varphi = 0 \} \cap D_{K_{12}}, \tag{B.2}$$

where

$$D_{K_{12}} = \{ \psi \in L^2(\Omega) : \psi|_{\partial\Omega} \in D(K_{12}) \subset \mathcal{H}_b \}. \tag{B.3}$$

Now suppose that K_{12} is self-adjoint on $N(P_{12})$. It may happen, in fact, that the sum $K_1 + K_2$ is not self-adjoint, and $D(K_1) \cap D(K_2)$ could even reduce to the trivial space! In particular, it is sufficient, for example, that either K_1 or K_2 is bounded, so that their sum is surely self-adjoint. The latter situation happens when, for example, 1 is in the resolvent set of V_{U_1} , that is when U_1 is gapped.

Then, by the representation theorem in [8] the form t_{12} is the expectation value of a self-adjoint operator, T_W (W being a unitary operator on \mathcal{H}_b), which is (half) the form sum operator of T_{U_1} and T_{U_2} , namely $T_W = (T_{U_1} + T_{U_2})/2$. Notice that, by the previous discussion it follows that T_W is bounded below because K_{12} is.

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