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# Casimir effect and global theory of boundary conditions

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## Abstract

The consistency of quantum field theories defined on domains with external borders imposes very restrictive constraints on the type of boundary conditions that the fields can satisfy. We analyse the global geometrical and topological properties of the space of all possible boundary conditions for scalar quantum field theories. The variation of the Casimir energy under the change of boundary conditions reveals the existence of singularities generically associated with boundary conditions which either involve topology changes of the underlying physical space or edge states with unbounded below classical energy. The effect can be understood in terms of a new type of Maslov index associated with the non-trivial topology of the space of boundary conditions. We also analyse the global aspects of the renormalization group flow, T-duality and the conformal invariance of the corresponding fixed points.

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## 1. Introduction

The role of boundaries in quantum physics has been boosted in the last decade until becoming a basic element of fundamental physics. The classical Weyl's dream of hearing the shape of a drum has been subsumed into a quantum dream of hearing the shape of a quantum drum or even a more dramatic one that of the shape of our universe.

In quantum mechanics the unitarity principle imposes severe constraints on the boundary behaviour of quantum states in systems restricted to bounded domains [1]. In relativistic field theories, causality imposes further requirements [2]. The space of boundary conditions compatible with both constraints has interesting global geometric properties. The dependence of many interesting physical phenomena, such as the Casimir effect [3], topology change [4] or renormalization group flows [5–7], on the boundary conditions can be analysed from this global perspective.

The effect of background fields in quantum theories has been extensively analysed from many perspectives. The induced dynamics on the background field by the effective action has many interesting implications [8, 9]. The analogue study with respect to possible boundary conditions has not been yet globally addressed, and this is the main purpose of this paper.

## 2. Self-adjointness boundary conditions

Let us for simplicity consider  $N$  massless free complex scalar fields  $\phi$  defined on a bounded domain  $\Omega$  with the smooth boundary  $\partial\Omega$ . The corresponding Hamiltonian is given by

$$\mathcal{H} = \frac{1}{2} \int_{\Omega} [|\pi_{\phi}|^2 + |\nabla\phi|^2 + m^2|\phi|^2] - \frac{1}{4} \int_{\partial\Omega} [\phi^{\dagger}\partial_n\phi - (\partial_n\phi^{\dagger})\phi], \quad (1)$$

where the boundary term is introduced to generate local classical equations of motion equation without requiring any specific type of boundary conditions [10, 11]. Indeed, the gradient term

$$\mathcal{V} = \frac{1}{2} \int_{\Omega} |\nabla\phi|^2 \quad (2)$$

can be rewritten as

$$\mathcal{V} = \frac{1}{2} \int_{\Omega} \phi^{\dagger}\Delta\phi + \frac{1}{2} \int_{\partial\Omega} \phi^{\dagger}\partial_n\phi, \quad (3)$$

where  $\partial_n$  denotes the normal derivative at the boundary  $\partial\Omega$ . If the space has a non-trivial Riemannian metric  $g$  the volume elements in the domain  $\Omega$  and its boundary  $\partial\Omega$  are

$$\delta\Omega = \sqrt{g}d^n x \quad \text{and} \quad \delta\partial\Omega = \sqrt{g_{\partial\Omega}}d^{n-1}x, \quad (4)$$

respectively.  $\Delta$  is the Laplace–Beltrami operator  $\Delta = -\nabla^{\mu}\partial_{\mu}$ .

In classical field theory, boundary conditions have to be imposed on the fields in order to find a unique solution of motion equations. In quantum theory, boundary conditions have to be imposed in order to preserve unitarity. In particular, the Laplace–Beltrami operator must be a self-adjoint operator. The standard theory of self-adjoint extensions due to von Neumann [12] establishes that there exists a one-to-one correspondence between self-adjoint extensions of  $\Delta$  and unitary operators from the deficiency spaces  $\mathcal{N}_+ = \ker(\Delta^{\dagger} + i\mathbb{I})$  to  $\mathcal{N}_- = \ker(\Delta^{\dagger} - i\mathbb{I})$ . There is, however, an alternative characterization [1] based on explicit constraints on boundary data which is more practical for physical applications. It establishes that the set  $\mathcal{M}$  of self-adjoint extensions of  $\Delta$  is in one-to-one correspondence with the group of unitary operators of the boundary Hilbert space  $L^2(\partial\Omega, \mathbb{C}^N)$ . For any unitary operator  $U \in \mathcal{U}(L^2(\partial\Omega, \mathbb{C}^N))$ , the fields satisfying the boundary condition<sup>1</sup>

$$\varphi - i\partial_n\varphi = U(\varphi + i\partial_n\varphi) \quad (5)$$

define a domain where  $\Delta$  is a self-adjoint operator.  $\varphi$  denotes the boundary value of  $\phi$  and  $\partial_n\varphi$  its normal derivative at the boundary. Although both characterizations are equivalent [1], the latter provides a group structure to the space  $\mathcal{M}$  of boundary conditions and allows a more direct analysis of its global properties.

In the case of open strings, for the corresponding conformal (1+1)-dimensional theories defined on the space interval  $\Omega = [0, 1] \subset \mathbb{R}$  we have  $\mathcal{M} = \mathcal{U}(2)$ . The unitary matrices

$$U_D = -\mathbb{I} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \quad U_N = \mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad U_P = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (6)$$

<sup>1</sup> Note that (5) is in general a non-local condition.  $U$  is any unitary operator in  $L^2(\partial\Omega, \mathbb{C}^N)$  that generically is non-local.

define Dirichlet, Neumann and periodic boundary conditions, which in string theory correspond to a string attached to a D-brane background, free open and closed string theories, respectively.

For higher  $N$ -dimensional target spaces, or  $N$ -component strings, the  $2N \times 2N$  matrices

$$U_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & \dots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \dots & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ 1 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \end{pmatrix} \quad U_N = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \dots & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \dots & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \dots & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \dots & 1 & 0 \end{pmatrix} \quad (7)$$

define self-adjoint extensions which correspond to one single closed string or  $N$  disconnected strings, respectively. The topology change is described in this way by a simple change of boundary conditions in  $\mathcal{M}$ .

### 3. Global topological structure of the space of self-adjoint boundary conditions

There are subsets of boundary conditions in  $\mathcal{M}$  where the constraint (5) acquires a simpler expression. If the spectrum of eigenvalues of the unitary operator  $U$  does not include the value  $-1$  (i.e.  $-1 \notin \text{Sp } U$ ) the boundary condition (5) can be rewritten as

$$\partial_n \varphi = -i \frac{\mathbb{I} - U}{\mathbb{I} + U} \varphi, \quad (8)$$

which means that only the boundary value of the fields at the boundary can have an arbitrary value  $\varphi$  whereas its normal derivative is determined by  $U$  and  $\varphi$ .

The corresponding operator mapping from unitary into self-adjoint operators

$$A = -i \frac{\mathbb{I} - U}{\mathbb{I} + U} \quad (9)$$

is the celebrated Cayley transform. The inverse Cayley transform

$$U = \frac{\mathbb{I} - iA}{\mathbb{I} + iA} \quad (10)$$

recovers the unitary operator  $U$  from its self-adjoint Cayley transform  $A$ .

If  $-1 \notin \text{Sp } U$  we can interchange the role of  $\varphi$  and  $\partial_n \varphi$ . In that case the boundary condition reads

$$\varphi = i \frac{\mathbb{I} + U}{\mathbb{I} - U} \partial_n \varphi. \quad (11)$$

However, there are two submanifolds (*Cayley submanifolds*) of  $\mathcal{M}$  defined by

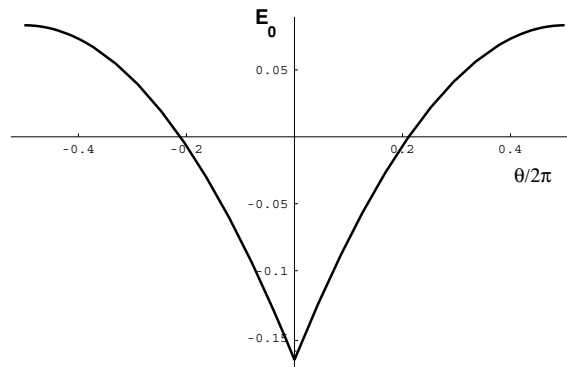
$$\mathcal{C}_\pm = \{U \in \mathcal{U}(L^2(\partial\Omega, \mathbb{C}^N)) \mid \pm 1 \in \text{Sp } U\} \quad (12)$$

where both transformations are singular.

The topology of the space  $\mathcal{M}$  of self-adjoint extensions is non-trivial,

$$\pi_1[\mathcal{U}(L^2(\partial\Omega, \mathbb{C}^N))] = \mathbb{Z} \quad (13)$$

and the Cayley submanifolds are homologically dual of the generating cycles of  $H_1(\mathcal{M})$  [1]. A generalized Maslov index can be defined for any closed path  $\gamma \in \mathcal{M}$  as the oriented sum of



**Figure 1.** Casimir energy for pseudo-periodic boundary conditions.

crossings of  $\gamma$  across the Cayley submanifold  $\mathcal{C}_-$ , i.e.

$$\nu_M(\gamma) = \int_0^{2\pi} \partial_\theta n(\gamma(\theta)) d\theta, \quad (14)$$

where  $n(\gamma(\theta)) = n_+(\gamma(\theta)) - n_-(\gamma(\theta))$  denotes the indexed sum of crossings of  $(\gamma(\theta'))$  for  $\theta' \leq \theta$ . A relevant consequence of the non-trivial structure of the space of boundary conditions is that a Berry phase can appear when the system follows a non-trivial closed loop in the space of boundary conditions.

Boundary conditions which correspond to the identification of points of the boundary can easily be identified because their unitary matrices  $U$  present pairs of eigenvalues  $\pm 1$ . The unitary operators associated with these boundary conditions belong to the intersection of the Cayley manifolds  $\mathcal{C}_+$  and  $\mathcal{C}_-$ . The transition from normal boundary conditions to any of these conditions involves a topology change. Now, such a topological transition always requires an infinite amount of classical energy [1]. This property follows from the fact that for any self-adjoint extension of  $\Delta$  with  $U \in \mathcal{C}_-$ , there exists a family of self-adjoint extensions with unitary operators  $U_t$  very close to  $U$  that have bounded edge states with negative classical energy  $E_-$  which diverges in the limit  $U_t \rightarrow U$ .

Classical fields with negative energy are possible if the Cayley transform operator  $A$  is not negative, because

$$\int_\Omega \phi^\dagger \Delta \phi = \int_\Omega |\nabla \phi|^2 - \int_{\partial\Omega} \phi^* A \phi. \quad (15)$$

However, non-positive self-adjoint extensions of  $\Delta$  might lead to inconsistencies in the quantum field theory if they are not bounded below by the mass term.

#### 4. Casimir energy and boundary conditions

The infrared properties of quantum field theory are very sensitive to boundary conditions [13]. In particular, the physical properties of the quantum vacuum state and the vacuum energy exhibit a very strong dependence on the type of boundary conditions. Let us consider, for simplicity, the case of a real massless field in 1+1 dimensions defined on a finite interval  $[0, L]$ .

For pseudo-periodic boundary conditions defined by the unitary operator

$$U_\theta = \cos \theta \sigma_x - \sin \theta \sigma_y, \quad \varphi(L) = e^{i\theta} \varphi(0) \quad (16)$$

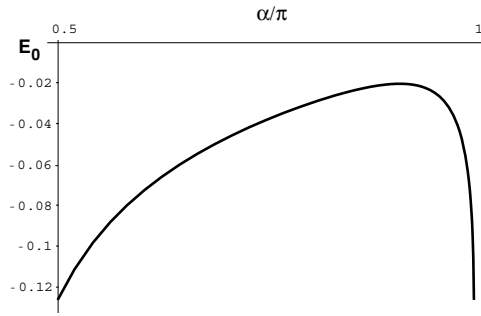


Figure 2. Vacuum energy for Robin boundary conditions.

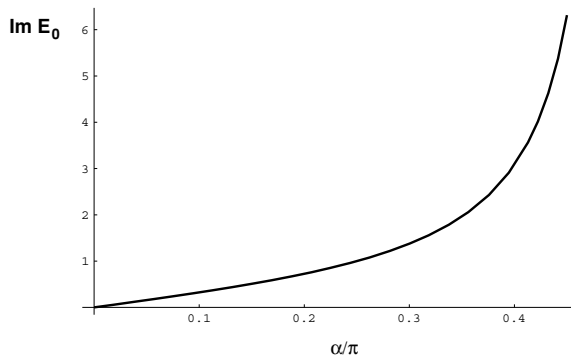


Figure 3. Behaviour of the imaginary term of the Casimir energy for Robin boundary.

the Casimir vacuum energy (see e.g. [14] and references therein) is given by (figure 1)

$$E_0 = \frac{\pi}{L} \left( \frac{1}{12} - \min_{n \in \mathbb{Z}} \left( \frac{\theta}{2\pi} + n - \frac{1}{2} \right)^2 \right). \tag{17}$$

The vacuum energy dependence in this case is relatively smooth. It presents a cuspidal point at  $\theta = 0$  which corresponds to periodic boundary conditions. A completely regular behaviour is obtained for Robin boundary conditions (figure 2)

$$U = e^{2\alpha i} \mathbb{I} \quad \partial_n \varphi(0) = \tan \alpha \varphi(0), \quad \partial_n \varphi(L) = \tan \alpha \varphi(L), \tag{18}$$

which smoothly interpolate between Dirichlet ( $\alpha = \frac{\pi}{2}$ ) and Neumann ( $\alpha = \pi$ ) boundary conditions when  $\alpha$  is restricted to the interval  $\alpha \in [\frac{\pi}{2}, \pi]$  [15–17].

However, the vacuum energy can exhibit more singular behaviours when globally considered as a function defined on  $\mathcal{M}$ . Indeed, for Robin boundary conditions (18) in the interval  $0 < \alpha < \frac{\pi}{2}$  the Casimir energy acquires an imaginary contribution due to the appearance of negative classical energy modes associated with edge states (figure 3).

The fact that the classical energy of this edge state becomes unbounded below when  $\alpha \rightarrow \frac{\pi}{2}$  implies a pathological behaviour of Casimir energy around the Dirichlet boundary condition point.

The existence of edge states giving rise to complex Casimir energies is a generic feature. For instance, the phenomenon also appears for Robin boundary conditions of the type

$$U = \begin{pmatrix} e^{2\alpha i} & 0 \\ 0 & e^{-2\alpha i} \end{pmatrix} \quad \partial_n \varphi(0) = \tan \alpha \varphi(0), \quad \partial_n \varphi(L) = -\tan \alpha \varphi(L) \tag{19}$$

except when  $\alpha = n\pi/2$ , which again correspond to Neumann and Dirichlet conditions [18]. In all the cases with imaginary vacuum energy the Hamiltonian

$$\mathcal{H} = \frac{1}{2}\sqrt{\Delta^U} \quad (20)$$

is not even a self-adjoint operator due to the existence of an edge estate of the self-adjoint operator  $\Delta^U$  with negative eigenvalue. The appearance of an imaginary part in the Casimir energy can be associated with a pair creation phenomenon. In all the above cases the imaginary term also becomes singular in the limit  $\alpha \rightarrow 0$  as a consequence of the AIM theorem [1]. However, the borderline regime  $\alpha = \frac{\pi}{2}$  is always very regular as corresponds to Dirichlet boundary conditions. The same phenomenon occurs around any boundary condition involving a topology change.

## 5. Boundary conditions and symmetries

The consistency of the quantum field theory imposes, thus, a very stringent condition on the type of acceptable boundary conditions even in the case of massive theories in order to prevent this type of pathological behaviour of vacuum energy.

Moreover, because of the existence of the boundary term in (1) the Hamiltonian  $\mathcal{H}$  (20) is not self-adjoint if the spectrum of the unitary operator  $U$  intersects the following domain of phase factors:

$$S_m^1 = \left\{ e^{2\alpha i}; -\pi < \alpha \leq \pi, 0 < \alpha < \frac{\pi}{2} - \arctan m^2, \text{ or } \frac{\pi}{2} < -\alpha < \pi - \arctan m^2 \right\}.$$

In any other case,  $-m^2$  is a lower bound for the spectrum of the operator  $\Delta^U$  and  $\mathcal{H}$  is self-adjoint.

The space of consistent boundary conditions for the quantum field theory

$$\mathcal{M}_m = \{U \in \mathcal{U}(L^2(\partial\Omega, \mathbb{C}^N)); \text{Sp } U \cap S_m^1 = \emptyset\} \quad (21)$$

is not necessarily multiple-connected, which means that we can have no Maslov index, although  $\mathcal{M}_m$  might also have a non-trivial topology.

For real scalar fields there is a further condition.  $U$  has to satisfy a CP symmetry preserving condition

$$U^\dagger = U^*, \quad U = U^T. \quad (22)$$

The usual Neumann and Dirichlet boundary conditions  $U = \pm \mathbb{I}$  satisfy this requirement. In general, for

$$U = \begin{pmatrix} A_1 & B \\ B^T & A_2 \end{pmatrix} \quad (23)$$

the condition requires that

$$A_1 = A_1^T, \quad A_2 = A_2^T, \quad A_1 B^* + B A_2^\dagger = 0 \quad (24)$$

$$B B^\dagger + A_1 A_1^\dagger = \mathbb{I}, \quad A_2 A_2^\dagger + B^T B^* = \mathbb{I}. \quad (25)$$

In particular, the quasi-periodic condition  $\varphi(L) = M^{-1}\varphi(0)$ ,  $\partial_n \varphi(L) = -M \partial_n \varphi(0)$  is also compatible if  $M = M^t = M^*$ .

In the case of a single real massless scalar the set of compatible boundary conditions is reduced from  $\mathcal{M} = S^3$  down to  $\mathcal{M} = \mathbb{Z}_2 \times nS^1$ , which also has a group structure and two connected components:  $\mathcal{M}_0$  given by the operators of the form  $U_\pm = \pm \mathbb{I}$  and  $\mathcal{M}_1$  given by

$$U_\alpha = \cos \alpha \sigma_z + \sin \alpha \sigma_x. \quad (26)$$

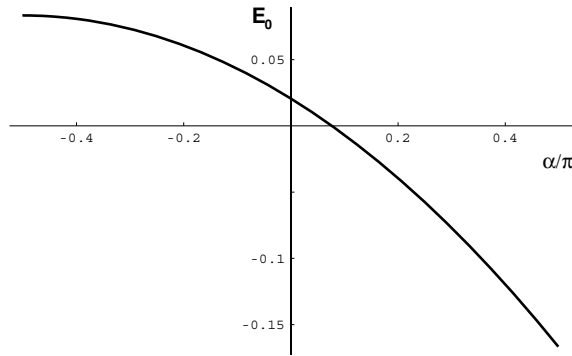


Figure 4. Casimir energy for quasi-periodic boundary conditions.

$\mathcal{M}_0$  includes Neumann and Dirichlet conditions, and  $\mathcal{M}_1$  contains the quasi-periodic boundary conditions

$$\varphi(L) = \tan \frac{\alpha}{2} \varphi(0); \quad \partial_n \varphi(L) = - \left( \tan \frac{\alpha}{2} \right)^{-1} \partial_n \varphi(0), \quad (27)$$

which include periodic ( $\alpha = \frac{\pi}{2}$ ) and antiperiodic ( $\alpha = -\frac{\pi}{2}$ ) boundary conditions.

In this case the topology of the global set of boundary conditions is not connected,  $\pi_0(\mathcal{M}) = \mathbb{Z}_2$ , and has a Maslov index,  $\pi_1(\mathcal{M}_1) = \mathbb{Z}$ .

The Casimir energy for quasi-periodic boundary conditions is [2]

$$E_0 = \frac{\pi}{L} \left( \frac{1}{12} - \min_{n \in \mathbb{Z}} \left( \frac{\alpha}{2\pi} + n + \frac{1}{4} \right)^2 \right), \quad (28)$$

(see figure 4).

Two particularly interesting cases of quasi-periodic boundary conditions are given by  $\alpha = 0$ ,

$$U_Z = \sigma_z; \quad \varphi(L) = 0, \quad \partial_n \varphi(0) = 0 \quad (29)$$

and  $\alpha = \pi$ ,

$$U'_Z = \sigma_z; \quad \varphi(0) = 0, \quad \partial_n \varphi(L) = 0, \quad (30)$$

which correspond to a Zaremba (mixed) boundary conditions: one boundary is Dirichlet and the other Neumann. In string theory they correspond to strings with one end attached to a zero-dimensional D-brane and the other free (see figure 5), which also can be thought as attached to a one-dimensional D-brane [19].

The vacuum energy of Zaremba boundary conditions

$$E_0 = \frac{\pi}{L} \left( \frac{1}{48} \right) \quad (31)$$

is slightly higher than that of a periodic boundary condition (closed string) and slightly lower than that of an antiperiodic boundary condition.

Note that the global analysis on  $\mathcal{M}$  permits us to understand a transition from a closed string to an open string with either DD, DN or NN boundary conditions [19]. However, as remarked above the transitions to DD or DN might involve an infinite amount of energy depending on the way the limit is obtained. The regularity of the interpolation (28) involving a topology change is a consequence of the fact that  $U_\alpha \in \mathcal{C}_- \cap \mathcal{C}_+$  for any value of  $\alpha$ .



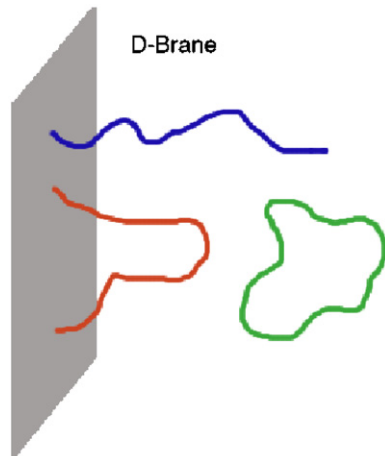


Figure 5. Different types of string attachments to a D-brane.

## 6. Conformal symmetry, renormalization group and T-duality

In 1+1 dimensions the classical theory of massless scalar fields is formally conformal invariant. However, the boundary term (1) might break this symmetry already at the classical level. In the quantum theory there is a conformal anomaly which makes the realization of conformal invariance more involved, even if the boundary condition is compatible with the symmetry.

In general, the boundary condition breaks conformal invariance and induces a renormalization group [5–7] flow in the space  $\mathcal{M}$  of boundary conditions (*boundary renormalization group flow*). Indeed, boundary conditions can be introduced into the action by means of a Lagrange multiplier,

$$\int_{\partial\Omega} \lambda(\varphi - i\partial_n\varphi - U[\varphi + i\partial_n\varphi]). \quad (32)$$

The renormalization of this boundary term defines the renormalization group of boundary conditions.

Conformal invariance is only preserved at the fixed points of this boundary renormalization group flow. These fixed points can easily be identified. Besides Dirichlet, Neumann and pseudo-periodic boundary conditions which obviously are conformal invariant, there are conditions such as quasi-periodic boundary conditions (26) which also preserve the conformal symmetry. In 1+1 dimensions they exhaust the whole set of conformal invariant boundary conditions. The topology of this subset of fixed points is  $\mathbb{Z}_2 \cup S^2 \cup S^2$  in the case of a charged scalar fields and  $\mathbb{Z}_2 \times nS^1$  in the case of neutral fields. In both cases the topology of the space of conformal invariant boundary conditions is still non-trivial.

All other boundary conditions flow towards any of these fixed points. The renormalization group behaviour around the fixed points is governed by the Casimir energy and presents different regimes. Dirichlet, Neumann and periodic boundary fixed points are stable whereas quasi-periodic and pseudo-periodic fixed points are in general unstable and marginally unstable, respectively.

For real scalar fields, Dirichlet, Neumann and periodic boundary conditions are the only stable points and the result holds for any dimension. The implications of this result in string theory are well known. Periodic boundary conditions appear as attractors of systems with

quasi-periodic and pseudo-periodic conditions which stress the stability of closed string theory vacuum.

For open strings the attractor (stable) points are standard free strings (Neumann) and strings attached to D-branes (Dirichlet). Any other boundary condition flows towards one of those fixed points.

In higher dimensions ( $n > 1$ ) the Hamiltonian (1) does not preserve conformal invariance even in the massless case  $m = 0$ . An extra term

$$\frac{n-1}{4n} \int \sqrt{g} R |\phi|^2 \quad (33)$$

proportional to the spacetime curvature  $R$  has to be added to the action. Conformal invariance also requires a similar modification of the Neumann condition in order to preserve conformal invariance

$$\partial_n \phi = \frac{n-1}{4n} K \phi, \quad (34)$$

where  $K$  is the extrinsic curvature of the boundary. Also more interesting boundary renormalization group flows arise. In the case of systems coupled to magnetic fields (e.g. Russian doll models) or with singular local interactions (see e.g. [20] for a review), fixed points with cyclic orbits of the boundary renormalization group flow can appear [21–23].

Finally, T-duality can also be globally defined in  $\mathcal{M}$ . Indeed, a T-transformation is defined by the involutive mapping of a theory with a boundary condition driven by an operator  $U$  into another theory driven by

$$U_T = -\sigma_2 U \sigma_2. \quad (35)$$

In particular, T transforms Dirichlet boundary conditions into Neumann boundary conditions and vice versa. Periodic boundary conditions are T-invariant. More generally, pseudo-periodic field theories  $U_\theta$  are transformed into pseudo-periodic theories  $U_{-\theta}$ . Note that in all cases T preserves the conformal invariant nature of the theory.

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