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Vacuum boundary effects

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Abstract

The effect of boundary conditions on the vacuum structure of quantum field theories is analysed from a quantum information viewpoint. In particular, we analyse the role of boundary conditions on boundary entropy and entanglement entropy. The analysis of boundary effects on massless free field theories points out the relevance of boundary conditions as a new rich source of information about the vacuum structure. In all cases the entropy does not increase along the flow from the ultraviolet to the infrared.

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1. Introduction

In quantum field theory the vacuum state encodes all physical properties of the theory. Indeed, any other state can be generated by the action of field operators on the vacuum. In particular, the effects generated by non-trivial topological structures of space or change of boundary conditions can be directly analysed from the changes induced on the vacuum structure. Among the most famous vacuum effects are the phenomenon of spontaneous symmetry breaking and the Casimir effect [1].

In particle physics, the main interest usually focuses on the behaviour of Green's and other quantum field correlation functions at short distances which provides information about high energy particle scattering processes. These observables are very insensitive to space topology or field boundary conditions [2]. However, for strongly correlated or confining theories long distance properties become very important, for instance, to point out the existence or not of confinement or mass gap. The existence of deconfining transitions in those theories (e.g. non-Abelian gauge theories) can be directly extracted from the analysis of the structure of the vacuum state. Another rich source of information about the theory is encoded in the behaviour of non-local observables such as free energy or entropy that can be defined by exploiting analogies with thermodynamics.

The interest on observables of this type has been recently boosted by the development of quantum information theory. The entanglement entropy [3] provides a good measure of the vacuum entanglement structure. It can also be used to point out the existence of phase transitions since it is unbounded for critical systems and bounded for systems with a finite mass gap [4]. It has been also pointed out that the confinement mechanism might be related to vacuum entanglement [5]. Another thermodynamic observable, the boundary entropy [6, 7] is related to the number of boundary states. Both new types of entropy do not scale with the volume of the space, unlike the standard bulk entropy and other extensive quantities. The entanglement entropy scales in the critical case with the area of the boundary where the fluctuating modes of the vacuum are traced out [3, 8]. This behaviour is characteristic of black hole physics and is one of the key features of the AdS/CFT correspondence.

By their own nature it is quite possible that both new entropies shall depend on the global properties of the configuration space. In this note we analyse the dependence of those quantities on the space topology and field boundary conditions as well as its physical implications for quantum field theories.

2. Boundary conditions and conformal invariance

Let us consider a real scalar free field theory defined in a bounded domain Ω in \mathbb{R}^D with regular and smooth boundary $\partial\Omega$. The quantum dynamics is governed by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \left\| \frac{\delta}{\delta\phi} \right\|^2 + \frac{1}{2} (\phi, \sqrt{-\Delta + m^2} \phi). \tag{1}$$

Unitarity requires that \mathcal{H} has to be self-adjoint. In particular, this implies that one must fix the boundary conditions of the fields ϕ in a way that the Laplace–Beltrami operator $-\Delta$ is self-adjoint and positive. The boundary conditions which define a self-adjoint operator $-\Delta$ are given by [9]

$$\varphi - i\dot{\varphi} = U (\varphi + i\dot{\varphi}) \tag{2}$$

in terms of an unitary operator $U \in \mathcal{U}(L^2(\partial\Omega, \mathbb{C}))$ which acts on the boundary values φ of the quantum fields ϕ and their normal derivatives $\partial_n\phi = \dot{\varphi}$. Notice that not all unitary operators give rise to positive Laplace–Beltrami operators, but to have a consistent quantum field theory for all values of m one needs to consider only boundary conditions which satisfy both requirements. The set of boundary conditions which are compatible with unitarity is given by unitary matrices U with eigenvalues $\lambda = e^{i\alpha}$ in the upper unit semi-circumference $0 \leq \alpha \leq \pi$. For a single real scalar field defined on the two-dimensional spacetime $\mathbb{R} \times [0, L]$ the set of compatible boundary conditions is a four-dimensional manifold which can be covered by two charts parametrized by

$$L \begin{pmatrix} \dot{\varphi}(0) \\ \dot{\varphi}(L) \end{pmatrix} = A \begin{pmatrix} \varphi(0) \\ \varphi(L) \end{pmatrix}, \tag{3}$$

where $A = -i(\mathbb{I} - U)/(\mathbb{I} + U)$ is any Hermitian matrix with $A \geq 0$, and

$$\begin{pmatrix} \varphi(L) \\ L\dot{\varphi}(L) \end{pmatrix} = B \begin{pmatrix} \varphi(0) \\ L\dot{\varphi}(0) \end{pmatrix}, \tag{4}$$

where $B = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is any real matrix with $ad + bc = -1$, $ac \leq 0$ and $bd \leq 0$.

In the massless case $m = 0$ the theory is conformally invariant. However, most of the compatible boundary conditions (3) and (4) break conformal invariance [6]. Only the boundary conditions corresponding to unitary matrices U with eigenvalues ± 1 preserve conformal

invariance [10, 11]. In the two-dimensional case the set of conformally invariant boundary conditions

$$\left\{ \mathbb{I}, -\mathbb{I}, U_\alpha = \begin{pmatrix} \cos \alpha & \sin \alpha \\ \sin \alpha & -\cos \alpha \end{pmatrix}; \alpha \in (0, 2\pi] \right\} \subset U(2), \quad (5)$$

is given by Neumann ($U = \mathbb{I}$), Dirichlet ($U = -\mathbb{I}$) and quasiperiodic (U_α) boundary conditions [10]. All other compatible boundary conditions break conformal invariance and are not invariant under renormalization group transformations. They describe renormalized trajectories of the renormalization group flowing towards one of the conformally invariant boundary conditions [11].

3. Boundary effects in conformal field theories

The infrared properties of quantum field theory are very sensitive to quantum field boundary conditions [2]. In particular, the physical properties of the quantum vacuum, free energy and vacuum energy exhibit a very strong dependence on the type of boundary conditions.

The vacuum state of the free field theory is gaussian

$$\Psi(\phi) = \mathcal{N} e^{-\frac{1}{2}(\phi, \sqrt{-\Delta+m^2}\phi)} \quad (6)$$

and the vacuum energy density $\mathcal{E}_0 = \text{tr} \sqrt{-\Delta+m^2}$ is ultraviolet divergent. However, for finite cylindric domains of the form $S^{D-1} \times [0, L]$ the finite size corrections ϵ_c of the asymptotic expansion of the vacuum energy density for large values of cylinder base radius Λ and generatrix L with $\Lambda \gg L \gg 1$

$$\mathcal{E}_0 = \epsilon_B + \epsilon_b \frac{1}{L} + \frac{1}{L^{D+1}} \epsilon_c(mL) + \mathcal{O}\left(\frac{1}{\Lambda}\right) \quad (7)$$

are not divergent [1]. In the massless limit $m \rightarrow 0$ the coefficient ϵ_c of this term becomes universal (i.e. independent of L) but is highly dependent on the boundary conditions¹. For instance, in two dimensions for quasiperiodic boundary conditions this first finite size correction is

$$\epsilon_c = \frac{\pi}{12} - \pi \left[\frac{\alpha}{2\pi} - \frac{3}{4} \right]^2. \quad (8)$$

The values and signs of this finite size contribution to the energy are very different for periodic ($\alpha = \pi/2, \epsilon_c = -\pi/6$), antiperiodic ($\alpha = 3\pi/2, \epsilon_c = \pi/12$) and Zaremba ($\alpha = \pi, \epsilon_c = \pi/48$) boundary conditions [13–18]. In higher dimensions we have for domains of the form $S^1 \times [0, L]$ the values of ϵ_c : $-\zeta(3)/(2\pi)$ for periodic, $3\zeta(3)/(8\pi)$ for antiperiodic and $3\zeta(3)/(64\pi)$ for Zaremba boundary conditions, where $\zeta(3) = 1.202\,0569$ is Apéry’s constant [19]. Similarly, in three-dimensional cylindric domains $S^2 \times [0, L]$ we have for the same boundary conditions $-\pi^2/90, 7\pi^2/720$ and $7\pi^2/11520$, respectively [19].

In a similar manner the free energy of the system at finite temperature $1/T$ with the boundary conditions (2) has the following asymptotic expansion for large volumes and low temperature $0 \ll L \ll T \ll \Lambda$ [7, 20],

$$f = -\frac{\log Z}{\Lambda^{D-1}L} = f_B T + f_b \frac{T}{L} + \frac{T}{L^{D+1}} f_c(mL) + \mathcal{O}\left(\frac{1}{T}, \frac{1}{\Lambda}\right), \quad (9)$$

where $f_B = \epsilon_B, f_b = \epsilon_b$ and $f_c = \epsilon_c$. This is in agreement with the asymptotic expansion of vacuum energy density (7) and for the same reason does not present any logarithmic dependence in the smaller transverse size scale L .

¹ The absence of logarithmic corrections $\mathcal{O}(\log L)$ is due to the topology of the boundary. In general those corrections spoil the universal character of the $\mathcal{O}(1)$ term [12].

In the asymptotic regime of low temperature and large volumes $0 \ll T \ll L \ll \Lambda$ we have

$$f = -\frac{\log Z}{\Lambda^{D-1}L} = f_B T + \frac{1}{T^D} \tilde{f}_c(mT) + \mathcal{O}\left(\frac{1}{L}, \frac{1}{\Lambda}\right). \quad (10)$$

There is a similar expansion for the entropy

$$S = (1 - T \partial_T) \log Z = -(D + 1) \frac{\Lambda^{D-1}L}{T^D} \tilde{f}_c(mT) + \frac{m\Lambda^{D-1}L}{T^{D-1}} \tilde{f}'_c(mT) + s_b + \mathcal{O}\left(\frac{1}{L}, \frac{1}{\Lambda}\right).$$

The third term of this expansion s_b , known as boundary entropy [6, 7], is finite and depends on the boundary conditions of the fields. In two-dimensional conformal theories this entropy $s_b = \log g$ can be formally associated with the number of boundary states g [6], but in many cases $g = e^{\log s_b}$ is not integer and does not correspond to a simple counting of boundary states [7]. It has been conjectured that the quantities g and s evolve with the renormalization group flow in a non-increasing way [7]

$$s_{UV} \geq s_{IR}, \quad g_{UV} \geq g_{IR}$$

as it corresponds to any type of thermodynamic entropy [7, 22]. This conjecture is known as g -theorem and has been verified in many cases [22, 23] although not yet proved for the boundary renormalization group flow.

The conjecture can be verified in the case of a two-dimensional free real scalar field defined on $\mathbb{R} \times [0, L]$. The partition function for antiperiodic boundary conditions, once properly renormalized, can be exactly calculated and it is given by

$$Z_a = q^{\frac{1}{24}} \prod_{n=1}^{\infty} (1 - q^{n-\frac{1}{2}})^{-2} = \frac{1}{2} \tilde{q}^{-\frac{1}{12}} \prod_{n=1}^{\infty} (1 - \tilde{q}^{2n-1})^2, \quad (11)$$

where $q = e^{-2\pi T/L}$ and $\tilde{q} = e^{-2\pi L/T}$. From (11) it follows that Casimir coefficient is in this case $\epsilon_c = \frac{\pi}{12}$. For Zarembo boundary conditions [24] we have

$$Z_z = q^{\frac{1}{96}} \prod_{n=1}^{\infty} (1 - q^{\frac{n}{2}-\frac{1}{4}})^{-1} = \frac{1}{\sqrt{2}} \tilde{q}^{-\frac{1}{12}} \prod_{n=1}^{\infty} (1 - \tilde{q}^{4n-2}), \quad (12)$$

which leads to the Casimir coefficient $\epsilon_c = \frac{\pi}{48}$.

For periodic boundary conditions there are zero modes which generate infrared divergences. The partition function (density) is given by [25]

$$z_p = \sqrt{\frac{L}{2\pi T}} q^{-\frac{1}{12}} \prod_{n=1}^{\infty} (1 - q^n)^{-2} = \sqrt{\frac{T}{2\pi L}} \tilde{q}^{-\frac{1}{12}} \prod_{n=1}^{\infty} (1 - \tilde{q}^n)^{-2}. \quad (13)$$

But, the infrared problem is so severe that affects the consistency of the theory [26]. In any quantum field theory the Schwinger functions must satisfy the Osterwalder–Schrader reflection positivity property in order to preserve unitarity and causality. However, in a free theory of two-dimensional massless bosons the two point function is neither positive nor reflection positive [27]. One way of solving all these problems is to consider a compactification of the scalar field $\Phi = e^{i\phi/R}$ to a circle of unit radius. In this case, the correlators of the compactified field Φ satisfy the reflection positivity requirement and theory becomes consistent [27].

In this case, the partition function acquires some additional contributions due to the compactification of zero modes. In particular, these contributions give rise to the following

partition function:

$$Z_p^R = q^{-\frac{1}{12}} \prod_{n=1}^{\infty} (1 - q^n)^{-2} \sum_{n,m=-\infty}^{\infty} q^{\pi R^2 n^2 + \frac{m^2}{4\pi R^2}} \quad (14)$$

$$= \tilde{q}^{-\frac{1}{12}} \prod_{n=1}^{\infty} (1 - \tilde{q}^n)^{-2} \sum_{n,m=-\infty}^{\infty} \tilde{q}^{\pi R^2 n^2 + \frac{m^2}{4\pi R^2}} \quad (15)$$

for periodic boundary conditions.

However, for the rest of quasiperiodic boundary conditions ($\alpha \neq \pi/2$) there is no contribution of the compactification of zero modes and the partition function is directly given by

$$Z_a^R = q^{\frac{1}{24} - \frac{1}{2}(\epsilon - \frac{1}{2})^2} \prod_{n=-\infty}^{\infty} (1 - q^{|n-\epsilon|})^{-1} \quad (16)$$

$$= \tilde{q}^{-\frac{1}{12}} (2 \sin \pi \epsilon)^{-1} \prod_{n=1}^{\infty} |1 - e^{2\pi i \epsilon} \tilde{q}^n|^{-2}, \quad (17)$$

where $\epsilon = \left| \frac{\alpha}{2\pi} - \frac{1}{4} \right|$. In particular, this means that for antiperiodic and Zaremba boundary conditions there is no modification of (11) and (12), respectively.

For Neumann boundary conditions the partition function is also modified by the presence of compact zero modes

$$Z_N^R = q^{-\frac{1}{48}} \prod_{n=1}^{\infty} (1 - q^{n/2})^{-1} \sum_{n=1}^{\infty} q^{\frac{n^2}{4\pi R^2}} \quad (18)$$

$$= \sqrt{\pi} R \tilde{q}^{-\frac{1}{12}} \prod_{n=1}^{\infty} (1 - \tilde{q}^{2n})^{-1} \sum_{n=1}^{\infty} \tilde{q}^{\pi R^2 n^2} \quad (19)$$

in a similar way that for the theory with Dirichlet boundary conditions, where

$$Z_D^R = q^{-\frac{1}{48}} \prod_{n=1}^{\infty} (1 - q^{n/2})^{-1} \sum_{m=-\infty}^{\infty} q^{\pi R^2 m^2} \quad (20)$$

$$= \frac{1}{2R\sqrt{\pi}} \tilde{q}^{-\frac{1}{12}} \prod_{n=1}^{\infty} (1 - \tilde{q}^{2n})^{-1} \sum_{m=-\infty}^{\infty} \tilde{q}^{\frac{m^2}{4\pi R^2}}. \quad (21)$$

The boundary entropy can easily be computed for all those cases and the results are

$$\begin{aligned} s_b^\alpha &= -\log (2 \sin \pi \epsilon) & g_\alpha &= (2 \sin \pi \epsilon)^{-1} & \text{quasiperiodic b.c.} \\ s_b^D &= -\log 2R\sqrt{\pi} & g_D &= (2R\sqrt{\pi})^{-1} & \text{Dirichlet b.c.} \\ s_b^Z &= -\frac{1}{2} \log 2 & g_Z &= 2^{-\frac{1}{2}} & \text{Zaremba b.c.} \\ s_b^N &= \log R\sqrt{\pi} & g_N &= R\sqrt{\pi} & \text{Neumann b.c.} \end{aligned} \quad (22)$$

The singularity observed for quasiperiodic boundary conditions at $\epsilon = 0$ is due to the existence of zero modes which once properly incorporated into the compact theory give rise to the correct value for periodic boundary conditions (14) and (15) with vanishing boundary entropy. Note also that $g_Z = \sqrt{g_D g_N}$ as corresponds to the factorization property of counting boundary states.

The g -theorem holds along the renormalized flow of Robin boundary conditions

$$U = \begin{pmatrix} e^{i\beta_0} & 0 \\ 0 & e^{i\beta_L} \end{pmatrix},$$

which interpolate between Dirichlet ($U = -\mathbb{I}$) and Neumann ($U = \mathbb{I}$) boundary conditions through Zaremba ($U = \sigma_3$) boundary conditions [28]

$$g_D > g_Z > g_N$$

provided that $R < 1/\sqrt{2\pi}$. The boundary entropy exhibits a monotone behaviour similar to that of the central charge or the bulk entropy.

4. Entanglement entropy

There is another type of entropy associated with the vacuum state of a field theory. If we ignore some field degrees of freedom of the theory one can consider the effective physical (mixed) states by tracing out those degrees of freedom. In this way mixed states with finite entropies can effectively appear in quantum field theory at zero temperature from pure states. The mechanism of tracing out degrees of freedom is a kind of quantum version of the renormalization group. In particular, the vacuum state generates by this mechanism a family of mixed states whose entropies provide measures of its degree of entanglement. These mixed states are generated by integration of the fluctuating modes of the vacuum state Ψ_0 in bounded domains Ω_1 of the physical space \mathbb{R}^D [3], i.e.

$$\rho_{\Omega_1} = \int_{\Omega_1} \Psi_0^* \Psi_0(x) d^D x. \tag{23}$$

The entropy of this state $S_{\Omega_1} = -\text{Tr} \rho_{\Omega_1} \log \rho_{\Omega_1}$ (vacuum entanglement entropy) is ultraviolet divergent, but once regularized exhibit a very interesting asymptotic behaviour which is similar to that of the boundary entropy analysed in the previous section [8, 22, 29–31]. For massless scalar theories the entropy presents the following asymptotic behaviour:

$$S_{\Omega_1} = \sum_{i=0}^{D-1} C_i \left(\frac{L_1}{a}\right)^i + \mathcal{O}\left(\frac{a}{L_1}\right), \tag{24}$$

in terms of the diameter L_1 of Ω_1 and the ultraviolet short distances cut-off a introduced to split apart the domain Ω_1 and its complement $\mathbb{R}^D \setminus \Omega_1$. In the three-dimensional case, this asymptotic behaviour follows an area law similar to the black hole area law [3, 8]. In general, for $D > 1$ the coefficients C_i are not universal because they are regularization dependent. However, for one-dimensional spaces, although the formula (24) suggests that C_0 could be universal, it does not happen. In fact, the asymptotic behaviour of the entanglement entropy is not given in that case by (24) because that entropy acquires a leading logarithmic correction

$$S_{\Omega_1} = C \log \frac{L_1}{a} + C_0, \tag{25}$$

which obviously implies that the constant term is highly dependent on the regularization method. However, it turns out that the value of the coefficient of this logarithmic term C is universal and equal to $1/3$ of the central charge c of the conformal invariant theory. In the case of a massless scalar boson $c = 1$ and $C = 1/3$ [32]. The question is whether this value is dependent or not on the boundary conditions of the fields when the theory is defined on a large bounded domain $\Omega \supset \Omega_1$. It is remarkable that coefficient $c_1 = 1/3$ turns out to be independent of the choice of boundary condition in $\Omega = (0, L)$ when $\Omega_1 = (L/2 - l/2, L/2 + l/2)$ is chosen to have half of the size of the interval. This result can be easily understood as a

consequence of the fact that the entanglement entropy is basically due to the behaviour of field correlations at the interface between Ω_1 and its complement $\Omega \setminus \Omega_1$ which does not involve the boundary values of the fields. On the other hand the finite part C_0 is highly dependent on the ultraviolet regularization method.

However, when Ω_1 reaches the boundary of the whole space Ω the entropy has the same asymptotic behaviour [33, 36]

$$S_l = \frac{C}{2} \log \frac{l}{\epsilon} + \log g + \frac{1}{2} C_0, \tag{26}$$

but with a different coefficient for the asymptotic logarithmic term and a different finite term which is related to the boundary entropy [7] and, thus also dependent on the boundary condition. The behaviour of this quantity along the boundary renormalization group flow has then the same monotone behaviour as the boundary entropy.

A similar phenomenon occurs in 2+1 dimensions with the constant term. In general, the entropy is given by

$$S_{\Omega_1} = C_1 \frac{L_1}{a} + C \log \frac{L_1}{a} + C_0. \tag{27}$$

The logarithmic term is absent for domains Ω and Ω_1 with smooth boundaries $\partial\Omega$ and $\partial\Omega_1$, whenever $\Omega \setminus \Omega_1$ is a connected manifold [37]. In a regularized theory the smoothness condition requires that the curvature of the boundaries must be always much larger than the ultraviolet cut-off a [38]. In that case, the remaining constant C_0 has a special behaviour because not only is regularization independent but also independent of the size of Ω_1 . C_0 can be split into two terms $C_0 = C'_0 + C_0^*$, one C'_0 which contains all possible dependences on the prescription used for the definition of the Ω_1 perimeter L_1 , and another one C_0^* which is absolutely prescription independent. In a massive theory, if L_1 is much larger than the inverse of the mass gap $1/m$, there is a prescription which uniquely fixes the ambiguities involved in such a splitting [39, 40]. If Ω_1 is decomposed as the disjoint union of three similar domains $\Omega_1 = \Omega_\alpha \cup \Omega_\beta \cup \Omega_\gamma$, one can define

$$C_0^* = C_0^{\Omega_1} - C_0^{\Omega_\alpha \cup \Omega_\beta} - C_0^{\Omega_\beta \cup \Omega_\gamma} - C_0^{\Omega_\alpha \cup \Omega_\gamma} + C_0^{\Omega_\alpha} + C_0^{\Omega_\beta} + C_0^{\Omega_\gamma}, \tag{28}$$

and the result is independent of the Ω_1 decomposition and the perimeter definition prescription. The constant C_0^* is also shape independent and only really depends on the topology of the domain $\Omega \setminus \Omega_1$. It defines a topological invariant entropy $S_{\text{top}} = C_0^*$ associated with the quantum vacuum [39, 40], which measures its degree of topological entanglement. It can be shown that $S_{\text{top}} = -\log \mathcal{D}$, where \mathcal{D} is the total quantum dimension of the underlying topological theory. In our case it is easy to show that $\mathcal{D} = 1$, which means the vanishing of the topological entanglement entropy, and that result is independent of the boundary conditions. In more general theories like the SU(2) WZWN theory with level k the topological entanglement entropy is given by [39]

$$S_{\text{top}} = \log \left[\sqrt{\frac{2}{k+2}} \sin \frac{\pi}{k+2} \right]. \tag{29}$$

The quantum dimension \mathcal{D} is non-integer in that case but it is a real topological invariant.

5. Conclusions

The novel thermodynamic quantities associated with field theories such as boundary entropy and vacuum entanglement entropy reveal new interesting properties of vacuum structure. The boundary entropy is associated with the existence of boundary states and, thus, is very sensitive

to the boundary conditions of the fields. The role of the vacuum entanglement entropy focuses on the measure of the amount of entanglement of the quantum vacuum and is absolutely independent of the type of boundary condition, whenever the domain where the quantum fluctuations of the fields are integrated out does not reach the boundary of the space. However, when this domain reaches the boundary, the entanglement entropy becomes dependent on the boundary conditions, displaying a monotone behaviour along the boundary renormalization group flow similar to that of the boundary entropy.

We have explicitly verified the behaviour of boundary and entanglement entropies under changes of boundary conditions for low dimensional massless free field theories. The boundary entropy varies for quasiperiodic boundary conditions and Robin boundary conditions, whereas the entanglement entropy only changes when the entanglement domain reaches the boundary or changes its topology. The same behaviour appears in three-dimensional field theories where the finite term of the asymptotic behaviour of the entanglement entropy can be related to a new topological invariant (topological entanglement entropy). For free scalar field theories we have shown that this topological invariant is trivial for connected convex domains, but self-interacting field theories and non-connected domains might have non-trivial topological entanglement entropy, which provides a basis for robust codes in quantum computation [39].

In all analysed cases the boundary entropy does not increase along the boundary renormalization group flow from the ultraviolet to the infrared [7, 28]. There are two interesting problems which remain open: the effect of interactions on both types of entropies associated with the quantum vacuum and their behaviour for topological field theories. Both problems deserve further analysis.

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