Holographic entanglement of purification near a critical point

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Abstract In the presence of finite chemical potential $\mu$, we holographically compute the entanglement of purification in a $2+1$- and $3+1$-dimensional field theory and also in a $3+1$-dimensional field theory with a critical point, at which a phase transition takes place. We observe that compared to $2+1$- and $3+1$-dimensional field theories, the behavior of entanglement of purification near critical point is different and it is not a monotonic function of $\frac{\mu}{T}$ where $T$ is the temperature of the field theory. Therefore, the entanglement of purification distinguishes the critical point in the field theory. We also discuss the dependence of the holographic entanglement of purification on the various parameters of the theories. Moreover, the critical exponent is calculated.

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1 Introduction

The AdS/CFT correspondence or more generally gauge-gravity duality (as an example of the holographic idea) opens a new window to study strongly coupled field theories. This duality enables us to describe and study various phenomena in the field theories utilizing their corresponding gravity duals. Although these phenomena may not seem simple from a field theory point of view, their gravitational descriptions hopefully have a simpler explanation. As an example, the confinement–deconfinement phase transition of quantum chromodynamics at low energy was highly discussed in the literature and it corresponds to the Hawking–Page phase transition on the gravity side [1]. Therefore, based on this idea the gravitational counterparts for different quantities in the field theory have been defined and thereby various properties of the field theory have been investigated.

As another example, in the context of quantum information theory, entanglement entropy is one of the most well-known quantities which has simple holographic dual. Entanglement entropy determines quantum entanglement between subsystems $A$ and its complementary for a given pure state. On the gravity side, it corresponds to the area of the minimal surface with a suitable condition at the boundary which is usually called Ryu and Takayanagi (RT)-surface [2–4]. This prescription has been frequently discussed and successfully passed a lot of non-trivial tests. Indeed, since in order to calculate entanglement entropy one only needs to compute an area, the calculation is much simpler in the gravity theory than in the strongly coupled field theory.

A new quantity which recently received a lot of interest in the gauge-gravity duality point of view is entanglement of purification (EoP) $E_p$. It measures correlations (quantum and classical) between two disjoint subsystems $A$ and $B$ for a given mixed state described by density matrix $\rho_{AB}$ where $AB = A \cup B$. Then, the EoP is defined as

$$E_p(\rho_{AB}) = \min_{\rho_{AB}=Tr_{A'B'}|\psi\rangle\langle\psi|} S_{AA'},$$

where $\rho_{AA'} = Tr_{BB'}|\psi\rangle\langle\psi|$, $S_{AA'}$ is the entanglement entropy associated with $\rho_{AA'}$ and the state $|\psi\rangle$ satisfies in the following conditions

- $|\psi\rangle \in \mathcal{H}_{AA'} \otimes \mathcal{H}_{BB'}$ where $A'$ and $B'$ are arbitrary. In fact by adding auxiliary degrees of freedom we construct a pure state, i.e. $|\psi\rangle$.
- $|\psi\rangle$s are pure states satisfy the condition $\rho_{AB} = Tr_{A'B'}|\psi\rangle\langle\psi|$ and therefore they are called purification of $\rho_{AB}$.

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Note that the minimization in (1) is taken over any pure states $|\psi\rangle$. It is then conjectured that the EoP is holographically dual to entanglement wedge cross-section $E_w$ of $\rho_{AB}$, as a measure of correlation between $A$ and $B$, which is defined [5,6]

$$E_w(\rho_{AB}) = \frac{\text{Area}(\Sigma_{AB}^{\text{min}})}{4G_N},$$

(2)

where $\Sigma_{AB}^{\text{min}}$ is the minimal area surface in the entanglement wedge $E_w(\rho_{AB})$ that ends on the RT-surface of $A \cup B$, the green line in 1 and $G_N$ is Newton’s constant. As a result, we have

$$E_p(\rho_{AB}) = E_w(\rho_{AB}).$$

(3)

Furthermore, it is also discussed in the literature that the entanglement wedge cross-section $E_w$ of $\rho_{AB}$ may be identified with logarithmic negativity [7], odd entropy [8], entanglement distillation [9] and reflected entropy [10]. The (logarithmic) negativity is a computable measure for quantum mixed states derived from the positive partial transpose criterion for the separability of mixed states and is defined by taking the trace norm of the partial transpose of the density matrix [7]. The odd entanglement entropy is a generalization of the entanglement entropy that measures the correlation between two subsystems in a mixed state. This quantity can be calculated by using the replica trick and enables us to compute the entanglement wedge cross-section in holographic CFTs [8]. The EoP of mixed states and therefore the entanglement wedge cross-section can be interpreted in terms of entanglement distillation [9]. The reflected entropy is defined for mixed quantum states and is the entanglement entropy associated with a canonical purification which is obtained by doubling the Hilbert space [10].

Using the prescription (3), some universal properties of EoP can be described holographically, for instance, see [5]. Moreover, it is also discussed that the EoP experiences a discontinuous transition when the two subsystems under study are distant enough. In addition, the above proposal generalizes to the time-dependent case and thereby quantum quenches have been studied [11]. Furthermore, in order to understand various aspects of the EoP, many papers appear in the literature, for example, see [12–16].

2 Calculating of the EoP in our models

In this paper, to compute the EoP, we would like to start with a general metric

$$ds^2 = f_1(r)dr^2 + f_2(r)dr^2 + f_3(r)d\bar{x}^2,$$

(4)

where $\bar{x} \equiv (x_1, ..., x_d)$. The above metric is asymptotically $\text{AdS}_{d+2}$ and $r$ is the radial direction. The strongly coupled field theory lives on the boundary at $r \to \infty$. $f_1$, $f_2$ and $f_3$ are arbitrary functions and will be fixed later on. We then consider two subsystems $A$ and $B$ at a given time slice as follows

$$x(r) \equiv x_l(r), \text{ where } x(r) \text{ is an odd function of } r,$$

$$-\frac{L}{2} \leq x_l \leq \frac{L}{2}, \quad i = 2, ..., d,$$

(5)

where the length of the both disjoint subsystems is equal to $l$ and $l'$ is distance between two subsystems, see Fig. 1. Thus for the case at hand it is easy to see that $\Sigma_{AB}^{\text{min}}$ runs along the radial direction and connects the minimum point of minimal surfaces $\Gamma_l$ and $\Gamma_{l+l'}$. Then, using (2), the area of this hypersurface turns out to be

$$E_w = \frac{L^{d-1}}{4G_N} \int_{r_{l+l'}}^{r_{l+l'}} dr \sqrt{f_2f_3^{d-1}},$$

(6)

where $r_{l+l'}^p$ and $r_{l+l'}^a$ denote the turning point of $\Gamma_l$ and $\Gamma_{l+l'}$, respectively. Clearly, due to the even symmetry of $x(r)$, the final result for the EoP does not depend on $x$. In order to find the value of the turning point, let’s say $r_{l+l'}^p$, we calculate the area of the following configuration

$$-\frac{l'}{2} \leq x(r) \equiv x_l(r) \leq \frac{l'}{2},$$

$$-\frac{L}{2} \leq x_i \leq \frac{L}{2}, \quad i = 2, ..., d,$$

(7)

which leads to

$$\text{Area} = 2L^{d-1} \int_{r_{l+l'}}^{r_{l+l'}} dr f_3^{d-1} \sqrt{f_2 - f_3 x(r)^2} \equiv \int dr \mathcal{L}.$$

(8)

Since $\mathcal{L}$ does not depend on $x$ explicitly, the corresponding Hamiltonian is constant and it is then easy to find

$$\frac{l'}{2} = \int_{r_{l+l'}}^{r_{l+l'}} dr \sqrt{\frac{f_2f_3^{d-1}}{f_3^2 - f_3^{d-1}}}.$$

(9)
where the constant is chosen to be $\sqrt{\frac{f_0(f_0 - f_{\phi}^{\prime})}{f_0^{\prime}}}$. The above equation, for a given value of $l'$, can be used to find $r_h^{l''}$, at least numerically. Similarly, one can find the value of $r_{2l'' + l'}$.

Now we are interested in studying the EoP near a critical point. Thus, the field theory we consider here is characterized by temperature $T$ and chemical potential $\mu$ and its $\mu - T$ phase diagram contains a first order phase transition line which ends in a critical point \cite{17, 18}. It is characterized by the ratio of $\frac{T}{\pi}$, as expected, since the underlying theory is conformal. Therefore, in 4+1 dimensions, we consider the following Lagrangian

$$L = \frac{1}{2G_N} \sqrt{-g} \left( \mathcal{R} - \frac{f(\phi)}{4} F_{\mu \nu} F^{\mu \nu} - \frac{1}{2} \left( \partial_{\mu} \phi \right)^2 - V(\phi) \right), \quad (10)$$

where

$$V(\phi) = - \left( 8 e^{\frac{\phi}{\sqrt{2}}} + 4 e^{-\sqrt{2} \phi} \right), \quad f(\phi) = e^{-2 \sqrt{2} \phi}. \quad (11)$$

g and $\mathcal{R}$ denote metric and its corresponding Ricci scalar. $F_{\mu \nu}$ is the field strength of the gauge field. $\phi$ is a scalar field and $V(\phi)$ is its potential. Then using the equations of motion, in the AdS radius unit, one can find \cite{17}

$$f_1(r) = - e^{2A(r)} h(r), \quad f_2(r) = \frac{e^{2B(r)}}{h(r)}, \quad f_3(r) = e^{2A(r)}, \quad (12)$$

where in this case of $d = 3$ and

$$A(r) = \ln \left( r \left( 1 + \frac{Q^2}{r^2} \right)^{\frac{1}{2}} \right),$$

$$B(r) = - \ln \left( r \left( 1 + \frac{Q^2}{r^2} \right)^{\frac{1}{2}} \right),$$

$$h(r) = 1 - \frac{M^2}{r^2 (r^2 + Q^2)}. \quad (13)$$

This metric describes a charged black hole background. $M$ is the black hole mass and $Q$ is its charge and its horizon is located at $r_h$. The latter can be obtained from $h(r_h) = 0$, leading to

$$r_h = \sqrt[4]{Q^4 + 4M^2 - Q^2}. \quad (14)$$

The temperature $T$ and chemical potential $\mu$ of the field theory, which is dual to metric (12), are given by

$$T = \frac{2r_h^2 + Q^2}{2 \pi \sqrt{Q^2 + r_h^2}}, \quad (15)$$

$$\mu = \frac{Q r_h}{\sqrt{Q^2 + r_h^2}}, \quad (16)$$

or equivalently

$$\frac{\mu}{T} = \frac{2 \pi \frac{Q}{r_h}}{2 + \left( \frac{Q}{r_h} \right)^2}. \quad (17)$$

As a result, it is easy to see that

$$T = T_0 \left( 1 + \frac{Q}{r_h} \right)^2 \left( \frac{\pi}{r_h} \right)^2, \quad (18)$$

where $T_0 = \frac{\mu}{T}$ denotes the temperature in the case of $Q \rightarrow 0$. The same equation in terms of field theory parameters is given by

$$T = T_0 \left[ \frac{\left( \frac{\mu}{T} \right)^2}{\left[ 1 + \frac{\left( \frac{\mu}{T} \right)^2}{\left( \frac{\pi}{r_h} \right)^2} \right]^{\frac{1}{2}}} \right]. \quad (19)$$

As expected $T \rightarrow T_0$ when $\mu \rightarrow 0$. One can easily check that the right hand side of above equation is a decreasing function of $\frac{\mu}{T}$ and hence it has minimum value near the critical point. We will back to this equation later on.

Having obtained $\frac{Q}{r_h}$ in the bulk solution with respect to $\frac{\mu}{T}$ in the boundary we will see that the background considered here contains two different branches of variables $\frac{Q}{r_h}$ corresponding to each value of $\frac{\mu}{T}$. It indicates the existence of a first order phase transition in field theory. The relation between parameters in the bulk and the parameters in field theory dual can be evaluated using (15)

$$\frac{Q}{r_h} = \sqrt{3} \left( 1 \pm \sqrt{1 - \frac{(\sqrt{3} \frac{\mu}{T})^2}{\sqrt{\frac{\pi}{r_h}^2 + \frac{\mu}{T}^2}}} \right). \quad (19)$$

Using the relations between entropy, $s$, and charge density, $\rho$, in terms of the bulk solution parameters $Q$ and $r_h$ one can evaluate the Jacobian $J = \frac{\partial (s, \rho)}{\partial (T, \mu)}$. If the Jacobian is positive
The EoP and $I/2$ with respect to $l'$ for $l = 0.5$ (left) and $l = 0.8$ (right).

In order to study the behavior of the EoP near the critical point and compare these results to the results for the field theory without critical point, we now consider RN-AdS $d+2$ metric which can be obtained from the following Lagrangian [19]

$$\mathcal{L} = \frac{1}{16\pi G_N} \sqrt{-g} \left( \mathcal{R} - F_{\mu
u} F^{\mu\nu} + d(d + 1) \right),$$

and using the equations of motion, one can find

$$ds^2 = -r^2 f(r) dt^2 + \frac{1}{r^2 f(r)} dr^2 + r^2 d\vec{x}^2,$$

$$f(r) = 1 - \frac{M}{r^{d+1}} + \frac{Q^2}{r^{2d}},$$

in the AdS radius unit. Comparing to (4), we have

$$f_1(r) = r^2 f(r) = \frac{1}{f_2(r)}, \quad f_3(r) = r^2.$$ (23)

Moreover, the above background contains a time component of the gauge field introduced. $M$ and $Q$ are the mass and the charge of the RN-AdS black hole, respectively. As usual, $r$ is radial coordinate and $r \to \infty$ is the AdS boundary. In addition, $\vec{x}$ are the $d$ dimensional coordinates at the boundary. The gauge-gravity duality indicates that the Hawking temperature of the black hole corresponds to the temperature of the gauge theory. The temperature of the RN-AdS$_{d+2}$ black hole is

$$T = \frac{r_h}{4\pi} \left( (d + 1) - (d - 1) \frac{Q^2}{r_h^d} \right).$$ (24)

Here $r_h$ is the radius of the event horizon, i.e. the largest root of $f(r) = 0$. The relation between $r_h$, $M$ and $Q$ is

$$M = r_h^{d+1} + \frac{Q^2}{r_h^{2d-1}}.$$ (25)

Moreover, the gauge-gravity duality provides a correspondence between the time component of gauge field at the boundary and the chemical potential in dual boundary gauge theory. Therefore, it turns out to be [19,20] i.e.

$$\mu = \sqrt{\frac{d}{2(d - 1)}} \frac{Q}{r_h^d}.$$ (26)
Fig. 4 The two top rows: the EoP with respect to $\frac{\mu}{T}$ for $l' = 0.1$. The two lower rows: half of the mutual information, $I_2$, with respect to $\frac{\mu}{T}$ for $l' = 0.1$ and different values of $l$. In the all of these diagrams $T$ is fixed and equal to 0.37.

Hence, it is easy to find that

$$\frac{\mu}{T} = \frac{1}{\sqrt{2(d-1)(d+1)r_h^2} - (d-1)Q^2}.$$  \hfill (27)

Using (6) and (22), one can easily find

$$E_p \equiv \frac{4G_N}{L^2}E_w = \int_{r_2}^{r_{2+l'}} dr \frac{r^{d-2}}{\sqrt{1 - \frac{M}{r^2\pi^2} + \frac{Q^2}{r^2}}}. \hfill (28)$$

Evidently, (20) and (28) reduce to the same equation in the limit of $Q \rightarrow 0$ and $d = 3$.

3 Numerical results

The mutual information $I$, which is a finite, positive, semi-definite quantity which measures the total correlation
between the two sub-systems A and B, is defined as \[ I(A, B) = S_A + S_B - S_{A\cup B} \] (29)

It is then well-known that in order to calculate entanglement entropy \( S_A, S_B \) and \( S_{A\cup B} \), one only needs to compute the RT-surface given by (8). Note that the lower limit of integral can be obtained from (9) for a given value of length.

In Figs. 2 and 3, we have checked the inequality between EoP and the mutual information, i.e.

\[ \frac{I}{2} \leq E_p, \] (30)

for the two subsystems A and B with the same length \( l \). These figures with different values of \( l \) and \( l' \) convince us that the above relation satisfies for all values of \( l \) and \( l' \). Clearly, when the mutual information is zero, the EoP is zero as well. Moreover, a phase transition between zero and non-zero values of EoP is observed.

We plot the EoP behavior in terms of \( \frac{\mu}{T} \) in Fig. 4. Although the value of EoP does not substantially depend on the \( \frac{\mu}{T} \), for small enough values of \( l \) a minimum value of the EoP appears at \( \frac{\mu}{T} = (\frac{\mu}{T})_{min} \). In fact, for \( \frac{\mu}{T} > (\frac{\mu}{T})_{min} \) \( (\frac{\mu}{T}) < (\frac{\mu}{T})_{min} \) the value of the EoP increases (decreases) and thus the EoP has a minimum value at \( (\frac{\mu}{T})_{min} \). Moreover, this figure indicates that there exist two values of \( \frac{\mu}{T} \) which have the same value of EoP near the critical point. Near the critical point, the value of EoP grows. Then, by raising \( l \) gradually, a maximum value for the EoP appears near the critical point. One should notice that there are values of \( l \) for which a maximum and minimum value of EoP exist, simultaneously. For large enough \( l \), the minimum disappears and as a result, the EoP has only a maximum at \( \frac{\mu}{T} = (\frac{\mu}{T})_{max} \).

In short, we conclude that

- The EoP is not a monotonic function of scale \( \frac{\mu}{T} \) and as a matter of fact, it experiences distinct behaviors. It can be an increasing or decreasing function of \( \frac{\mu}{T} \) depending on the values of \( l \) and \( l' \) and not \( l/ l' \). It is clear that the non-trivial behavior of EoP depends on the values of \( l \) and \( l' \), though we cannot find their dependence analytically.
- The value of \( \frac{\mu}{T} \) at which the EoP achieves its maximum or minimum depends on the \( l \) and \( l' \), as it is expected.
- In the presence of the chemical potential, the EoP can decrease or increase. In other words, the correlation between two systems becomes stronger or weaker depending on the value of \( \frac{\mu}{T} \).
- Inequality (30) always satisfies (up to our numerical calculation).

An interesting observation of the EoP is that for given values of the subsystems and their separation there are two or three different configurations, labeled by various values of \( \mu/T \) s, with the same EoP. In fact, for given values of \( l \) and \( l' \), when the system is described by a mixed state characterized by \( \mu/T \), the correlation between the subsystems can be equal independent of \( \mu/T \). It is then instructive to investigate that this behavior takes place because of the existence of the critical point in the field theory.

In order to check this claim, we consider another charged black hole background corresponding to a field theory in the presence of chemical potential without a critical point. This background has been introduced in (22). We then plot the EoP in terms of \( \frac{\mu}{T} \) in Fig. 5 using the backgrounds metrics (12) (left panel) and (22) with \( d = 3 \) (right panel). First of all, it is clearly seen that when \( l \) and \( l' \) are kept fixed there are many points with different values of \( \frac{\mu}{T} \) which have the same value of EoP. From the gauge theory point of view, it means that there exists many mixed states with the same correlation between two subsystems independent of \( \frac{\mu}{T} \). It is an important
result. Although the states under study are not the same, since they have different values of $\mu$ and $T$, the correlation between two subsystems is identical. Moreover, when $\mu$ ($T$) is kept fixed the EoP decreases (increases) by decreasing temperature (increasing chemical potential). Equivalently, by raising the temperature the correlation increases meaning that the distance between subsystems becomes larger. Furthermore, notice that the EoP has the minimum value at the critical point, see Figs. 7 and 8.

We also consider the background (22) with $d = 2$. The EoP, (28) with $d = 2$, in terms of $\frac{\mu}{T}$ and $l'$ has been plotted in Fig. 9. Our results are similar to the case of $d = 3$ and we do not report them here. However, the left panel of above figure shows an opposite treatment compared to the 3 + 1-dimensional field theories.

In Fig. 10, as it was mentioned already, we assume that the slope of EoP with respect to $\frac{\mu}{T}$ changes as ($(\frac{\mu}{T})_s - \frac{\mu}{T})^{-\theta}$ where $\theta$ is the critical exponent obtained to be equal to 0.5 in [17] using Kubo commutator for conserved currents and confirmed in [18,22,23] by using quasinormal modes, equilibration time and saturation time, respectively. Therefore, we define

$$\frac{dE_p}{d(\frac{\mu}{T})}(i) = \frac{E_p(i + 1) - E_p(i)}{\frac{\mu}{T}(i + 1) - \frac{\mu}{T}(i)},$$

where $i$ refers to the number of numerical data points. Our results indicate that although the quantity we consider here is basically different with above mentioned papers, the value of the critical exponent is around 0.5, i.e. 0.534 and 0.526 for the left and right panel of Fig. 10, top row. To obtain these two numbers, we also plot the linear log-log diagram for which the critical exponent is the slope of a line, i.e. $\log(\frac{dE_p}{d(\frac{\mu}{T})}) \propto \log((\frac{\mu}{T})_s - \frac{\mu}{T})$. In order to report how well our fitted $\theta$ is we calculate relative error (RE) and root mean square (RMS) which are defined as

$$RE = \frac{|\theta - 0.5|}{0.5},$$

$$RMS = \sqrt{\frac{1}{N} \sum(y_{fit} - y_{data})^2},$$

where $y_{fit}$ is the value of fitted function $y$ evaluated at data points $x$ and $y_{data}$ is the corresponding value read from
Fig. 7 Left: the EoP with respect to $l$ for three different values of $\mu_T$ and $l' = 0.3$ in the field theory with a critical point. Right: the EoP with respect to $l$ for the same values of $\mu_T$ and $l'$ with non-zero chemical potential corresponding to (22) with $d = 3$. In both figures, the well-known phase transition between zero and non-zero mutual information, or equivalently the EoP, is shown by the dashed line. The three different values of $\mu_T$ are chosen to have the same $T$ equal to 0.37 and different $\mu$.

Fig. 8 The EoP with respect to $l'$ for $l = 0.8$. The left (right) panel has been plotted for the field theories dual to (12) ((22) with $d = 3$). The three different values of $\mu_T$ are chosen to have the same $T$ equal to 0.37 and different $\mu$.

Fig. 9 Left: the EoP with respect to $\mu_T$ for $l' = 0.1$, $l = 0.5$ in 2 + 1-dimensional field theory. The blue and green points show $T = 0.459$ and $\mu = 0.508$, respectively. Middle: the EoP with respect to $l$ for $l' = 0.3$ in 2 + 1-dimensional field theory. Right: The EoP with respect to $l'$ for $l = 0.8$ in 2 + 1-dimensional field theory. The three different values of $\mu_T$ are chosen to have the same $T$ equal to 0.21 and different $\mu$.
data and $N$ is the number of data points. These numbers are reported in the caption of Fig. 10.

A similar analysis for the mutual information can be used to find $\theta$. In other words, as one can see in Fig. 10, bottom row, we plot $dI/d(\mu_T)$ in terms of $\mu_T$. The outcomes indicate that the value of $\theta = 0.5$ is a good approximation. We would also like to mention that the behavior of mutual information near the critical point has been discussed analytically in [24] and their results show that $\theta = 0.5$.

Furthermore, using (18), the derivative of $T_0/T$ with respect to $\mu_T$ can be obtained

$$
\frac{d(T_0/T)}{d(\mu_T)} = \left( (\frac{\mu}{T}) (\frac{\mu}{T}) - \frac{\pi}{2} \right) - \frac{\pi}{4} + \mathcal{O}\left( \left( \frac{\mu}{T} \right) - \frac{\mu}{T} \right)
$$

(33)

This equation indicates that $d(T_0/T)/d(\mu_T)$ diverges near the critical point and therefore we expand (33) in power of $(\mu/T)_s - \mu/T$.

which is a measure of deviation from the critical point. We then have

$$
\frac{d(T_0/T)}{d(\mu_T)} = -\left( (\frac{\mu}{T})_s - \frac{\mu}{T} \right)^{-\frac{1}{2}} + \mathcal{O}\left( \left( \frac{\mu}{T} \right)_s - \frac{\mu}{T} \right)
$$

(34)

and thus $\theta = 0.5$. Moreover, we plot the EoP with respect to $T_0/T$. Note that Fig. 11 show that the EoP is not a monotonic function of $T_0/T$.

As the last point, we would like to mention that it seems since the critical exponent is a property of the background or equivalently of the gauge theory, its value is insensitive to the static observables. Therefore, as long as the field theory is probed by static observables the same result is obtained. However, this argument is not always correct and it is violated by dynamical probe, for instance, see [22]. In this paper, it is shown that the value of the critical point is not equal to 0.5 anymore and depends on the time scale of energy injection.
The EoP as a function of $\frac{T_1}{T}$ for $l' = 0.1$ and different values of $l$. $T$ is fixed and equal to 0.37.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors’ comment: This is a theoretical study and no experimental data.]

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