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Entanglement quantifiers, entanglement crossover and phase transitions

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Abstract. Entanglement has been widely used as a tool for the investigation of phase transitions (PTs). However, analysing several entanglement measures in the two-qubit context, we see that distinct entanglement quantifiers can indicate different orders for the same PT. Examples are given for different Hamiltonians. This leaves open the possibility of addressing different orders to the same PT if entanglement is used as an order parameter. Moving on to the multipartite context, we show necessary and sufficient conditions for a family of entanglement monotones to confirm quantum PTs.

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Contents

1. Introduction

The study of phase transitions (PTs) from the viewpoint of exclusively quantum correlations has captured the interest of the quantum information community recently [1, 2]. Linking entanglement and (quantum) PTs is tempting since PTs are related to long-range correlations among the system's constituents [3]. Thus expecting that entanglement presents a peculiar behaviour near criticality is natural.

Recent results have shown a narrow connection between entanglement and critical phenomena. For instance, bipartite entanglement has been widely investigated close to singular points and has exhibited interesting patterns [1, 2]. The *localizable entanglement* [4] has been used to show certain critical points that are not detected by classical correlation functions [5]. The *negativity* and the *concurrence* quantifiers were shown to be quantum-PTs witnesses [6]. Furthermore, the transitions between a normal conductor and a superconductor and between a Mott-insulator and a superfluid exhibit close relations between entanglement and the order parameters usually associated with it [7]. The main route that has been taken is the study of specific entanglement quantifiers for some chosen systems, but the general feeling is that a profound relation may appear.

In this paper, we go further in this direction starting from the generic result that, for a bipartite (finite) system at thermal equilibrium with a reservoir, there exist two distinct phases, one in which some entanglement is present and another one where quantum correlations completely vanish. We then exemplify this result with two-qubit systems subjected to different Hamiltonians. It is found that different entanglement quantifiers show distinct features for this *entanglement crossover*. This shows that if one uses different quantifiers to characterize a PT—for example, through a reduced state of an infinite chain [1, 2, 6, 7])—it is possible to attribute different orders to this phenomenon.

Although multipartite entanglement also plays an important role in many-body phenomena (it is behind some interesting effects such as the *Meissner effect* [8], *high-temperature superconductivity* [9], and *superradiance* [10]), rare results linking it to PTs are available. Crossing this barrier is also a goal of this paper. For that, we give necessary and sufficient conditions for a large class of multipartite entanglement quantifiers to signal singularities in the ground state energy of the system. We finish this work by discussing a recently introduced quantum PT, the *geometric PT*, which takes place when singularities exist at the boundary of the set of entangled states.

A PT occurs when some state function of a system presents two distinct phases, one with a non-null value and another one in which this function takes the null value [11]. Such a function is

called an *order parameter* for the system. However one can regard this as a very tight definition and want to define a PT as a singularity in some state function of the system due to changes in some parameter (coupling factors in the Hamiltonian, temperature, etc). By extension, this function is also called the order parameter of the PT.[5] Note that the first definition of PT is a special case of the latest one. When the singularity expresses itself as a discontinuity in the order parameter it is said that we are dealing with a discontinuous PT. If the discontinuity happens in some of the derivatives of the order parameter, say the nth-derivative, it is said to be a nth-order PT, or a continuous PT. In this paper, we will consider entanglement as a state function and see that it can present a singularity when some parameter of the problem changes. Thus, we give a more general discussion about when a given entanglement quantifier, or some of its derivatives, can present a discontinuity.

2. The entanglement crossover

It has been recently verified that an entanglement crossover is behind several PT, including those in interesting models like Bose–Hubbard [7], η-pairing [9] and Dicke [10]. Effects such as superradiance and superconductivity were shown to be closely related to the appearance of quantum correlations in the systems. It then became natural to study the so-called *entanglement crossover*, i.e., the crossing of a border between an entangled and a separable phase [12]. Curiously it is possible that systems exhibit various entanglement crossovers when heated [13]. In this section, we join this effort and investigate the entanglement crossover of systems in thermal equilibrium with a reservoir. Roughly speaking, the systems display two distinct phases: one separable and other entangled. Then the following question arises: is this transition smooth? We will show that the answer for this question depends on the adopted entanglement quantifier.

Let us first revisit a general result following from a simple topological argument. Given a quantum system with Hamiltonian H, its thermal equilibrium state at absolute temperature T is given by $\rho(T) = Z^{-1}\exp(-\beta H)$, where $Z = \mathrm{Tr}\,\exp(-\beta H)$ is the partition function and $\beta = (k_\mathrm{B}T)^{-1}$, k_B denoting the Boltzmann constant. This state is a continuous function of its parameters. If the space state of the system has finite dimension d, then $\lim_{T\to\infty}\rho(T) = I/d$, where I denotes the identity operator. For multipartite systems, I/d is an interior point in the set of separable states [14], i.e., it is separable and any small perturbation of it is still a separable state. Thus the one parametric family of thermal equilibrium states $\rho(T)$ can be viewed as a continuous path on the density operators set, ending at I/d. So if for some temperature T_e the state $\rho(T_\mathrm{e})$ is non-separable, there is a finite critical temperature $T_\mathrm{c} > T_\mathrm{e}$ (the crossover temperature) such that $\rho(T_\mathrm{c})$ is in the boundary of the set of separable states. An important class of examples is given by the systems with entangled ground state[6], i.e., $T_\mathrm{e} = 0$.

[5] Sometimes the order parameter is not a measurable property of the system, but we do not want to enter into this aspect.

[6] Bipartite systems with factorizable ground states can have thermal equilibrium states separable for all temperatures, or can also show entanglement at some temperature. In this case, there will be (at least) two PTs when temperature is raised: one from separable to entangled, and another from entangled to separable [2]. Also multipartite versions of this theorem can be stated: for each kind of entanglement which the system shows at some temperature, there will be a finite temperature of breakdown of this kind of entanglement.

It is clear that the entanglement E of the system will present a singularity at T_c. Let us focus more attention on the result that 'thermal-equilibrium entanglement vanishes at finite temperature' [12, 15]. It will be shown that different entanglement quantifiers deal differently with the same crossover. For that we will show an entanglement quantifier that is discontinuous at T_c, two others presenting a discontinuity at its first derivative, and another one in which the discontinuity manifests itself only in $\mathrm{d}^2E(\rho)/\mathrm{d}T^2|_{T=T_c}$.

As the first example take the Indicator Measure, $\mathrm{IM}(\rho)$, defined as one for entangled states and zero for separable ones. Although IM is an entanglement monotone[7], it is quite weird once it is a discontinuous function itself. Of course IM presents a discontinuity at $T = T_c$, i.e., when ρ crosses the border between the entangled and the disentangled-states world.

Let us now focus on some more interesting and natural entanglement quantifiers, namely the concurrence C, the entanglement of formation E_f, and the negativity N. These three functions are able to quantify entanglement properly although, as will be seen, in different ways[8]. The entanglement of formation was proposed by Bennett *et al* [17] as the infimum of mean pure state entanglement among all possible ensemble descriptions of a mixed state ρ. The concurrence was developed by Wootters and collaborators [18] in the context of trying to figure out a feasible way to calculate the entanglement of formation. Thus E_f and C are connected by

$$E_f(\rho) = H_2(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{1 - C^2(\rho)}), \tag{1}$$

where $H_2(x) = -x \log x - (1-x)\log(1-x)$ and it is assumed that $0 \log 0 = 0$. The concurrence can be defined by

$$C(\rho) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4), \tag{2}$$

with λ_i being the square roots of the eigenvalues of the matrix $\rho(\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$ in decreasing order and σ_y is the Pauli matrix.

On the other hand, the negativity uses the idea of partial transpose to calculate entanglement [14, 19]. It can be defined as

$$N(\rho) = \|\rho^{T_A}\| - 1, \tag{3}$$

where the subscript T_A indicates the partial transpose operation and $\|\star\|$ means the trace norm. Alternatively, one can define the logarithmic negativity as [14, 19] $E_{\mathcal{N}}(\rho) = \log_2(1 + N(\rho))$.

Let us use these quantifiers to study the entanglement of thermal-equilibrium states,

$$\rho = \frac{\exp(-\beta H)}{Z}, \tag{4}$$

subject to a completely non-local Hamiltonian of the form [20]

$$H = x\sigma_x \otimes \sigma_x + y\sigma_y \otimes \sigma_y + z\sigma_z \otimes \sigma_z. \tag{5}$$

[7] Entanglement monotones are quantifiers that do not increase when LOCC-operations are applied in ρ [16]. This feature has been viewed by many people as the unique requirement for a good quantifier of entanglement.

[8] In this section, we deal only with two-qubit systems. As in this case there is no PPT-entanglement, negativity becomes a good entanglement quantifier and an indicator of cross-overs. Also, the definition of the concurrence here shown is the original one, tailored by these systems, and not one of its further generalizations.

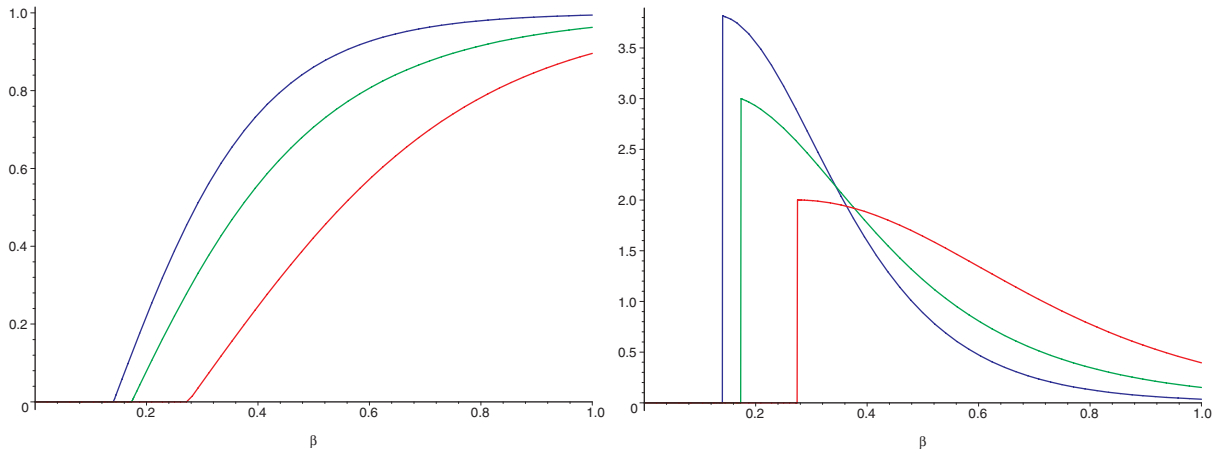

Figure 1. Left panel: $C(\rho)$ versus β for $x = 1$, $y = 1$, $z = 1$ (red); $x = 3$, $y = 1$, $z = 1$ (green); and $x = 3$, $y = 2$, $z = 1$ (blue). Right panel: $\mathrm{d}C(\rho)/\mathrm{d}\beta$ versus β for the same values of x, y, and z. Discussions on the figures are in the text. C shows a crossover of first-order (its first derivative is discontinuous). In the cases considered $C(\rho) = N(\rho)$, and the conclusions are also valid for the negativity [21].

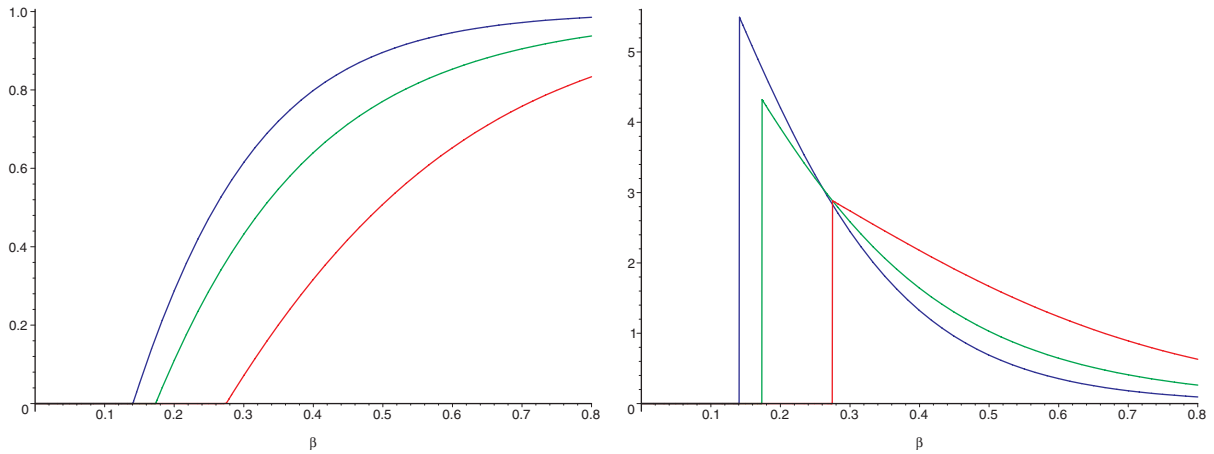

Figure 2. Left panel: $E_{\mathcal{N}}(\rho)$ versus β for $x = 1$, $y = 1$, $z = 1$ (red); $x = 3$, $y = 1$, $z = 1$ (green); and $x = 3$, $y = 2$, $z = 1$ (blue). Right panel: $\mathrm{d}E_{\mathcal{N}}(\rho)/\mathrm{d}\beta$ versus β for the same values of x, y and z.

Note that the usual one-dimensional (1D) two-qubit Heisenberg chains are particular cases of (5) (e.g., the XXX model holds when $x = y = z = J$, $J < 0$ being the ferromagnetic and $J > 0$ the antiferromagnetic cases). The results are plotted in figures 1–3.

From the figures we see that while the concurrence, the negativity, and the logarithmic negativity exhibit an abrupt crossover, the entanglement of formation smooths this transition. This leads us to the conclusion that if one uses the entanglement of a system as the order parameter of a PT, the attributed order is different according to the chosen quantifier. In our examples E_{f} would attribute a second-order transition, while according to C, N, and $E_{\mathcal{N}}$ it would be of first order, and remember that according to IM all transitions are discontinuous. In fact, it is possible to

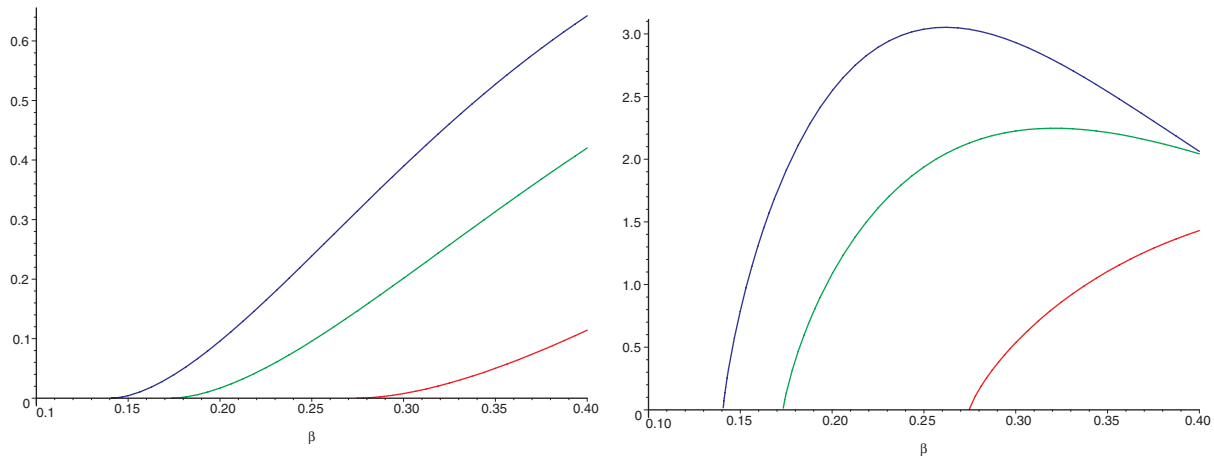

Figure 3. Left panel: $E_{\mathrm{f}}(\rho)$ versus β for $x = 1$, $y = 1$, $z = 1$ (red); $x = 3$, $y = 1$, $z = 1$ (green); and $x = 3$, $y = 2$, $z = 1$ (blue). Right panel: $\mathrm{d}E_{\mathrm{f}}(\rho)/\mathrm{d}\beta$ versus β for the same values of x, y and z.

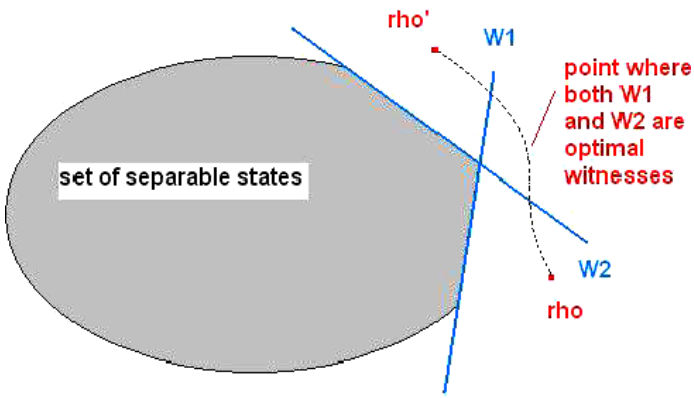

Figure 4. The dot (red) line represents the way followed by ρ when some parameter of the system is changed. Geometrically, entanglement witnesses can be interpreted as tangent hyperplanes to S_k. At a certain point both witnesses $W1$ and $W2$ are optimal for ρ. At this point, there is a singularity in $E_{\mathrm{W}}(\rho) = -\mathrm{Tr}(W_{1or2}\rho)$.

see, directly from its definition, that $E_{\mathcal{N}}$ will always present a discontinuity in the same derivative as N. For this aim, we can write:

$$\frac{\mathrm{d}E_{\mathcal{N}}(\beta)}{\mathrm{d}\beta} = \frac{1}{(1 + N(\beta))\ln 2}\frac{\mathrm{d}N(\beta)}{\mathrm{d}\beta}. \tag{6}$$

Similarly, the relation between E_{f} and C can be also verified analytically. The derivative of E_{f} with respect to β is

$$\frac{\mathrm{d}E_{\mathrm{f}}(\beta)}{\mathrm{d}\beta} = \frac{C(\beta)}{2\sqrt{1 - C^2(\beta)}}\log\left(\frac{1 - \sqrt{1 - C^2(\beta)}}{1 + \sqrt{1 - C^2(\beta)}}\right)\frac{\mathrm{d}C(\beta)}{\mathrm{d}\beta}. \tag{7}$$

So it is possible to see that, even with $C(\beta)$ being singular at ρ_c (it is, when $T = T_{\mathrm{c}}$), the singularity manifests itself on $E_{\mathrm{f}}(\beta)$ only to the next order.

In fact, this situation resembles that in percolation theory, when different 'percolation quantifiers' like probability of percolation, the mean size of the clusters, and the conductivity between two points show different critical behaviour [22].

3. Multipartite entanglement as indicator of quantum PTs

In [6], it is shown that the concurrence and the negativity serve themselves as quantum-PT indicators. The argument is that, avoiding artificial occurrences of non-analyticities, these quantifiers will present singularities only if a quantum PT happens. Further results for other bipartite entanglement quantifiers are presented in [23]. In the same context, Rajagopal and Rendell [24] offer generalizations of this theme to the more general case of mixed states.

By following the same method, we now extend the previous results to the multipartite case. We will see that it is possible to establish some general results, similar to [6], also in the multipartite scenario. We can use for this aim the *Witnessed Entanglement*, $E_{\mathrm{W}}(\rho)$, to quantify entanglement [25] (this way of quantifying entanglement includes several entanglement monotones as special cases, such as the robustness and the best separable approximation measure). Before giving the definition of E_{W}, we must review the concept of entanglement witnesses. For any entangled state ρ, there is an operator that witnesses its entanglement through the expression $\mathrm{Tr}(W\rho) < 0$ with $\mathrm{Tr}(W\sigma) \geqslant 0$ for all k-separable states σ (we call k-separable every state that does not contain entanglement among any $m > k$ parts of it, and denote this set S_k) [25]. We are now able to define E_{W}. The witnessed entanglement of a state ρ is given by

$$E_{\mathrm{W}}^{k}(\rho) = \max\left[0, -\min_{W\in\mathcal{M}} \mathrm{Tr}(W\rho)\right], \tag{8}$$

where the choice of $\mathcal{M}$ allows the quantification of the desired type of entanglement that ρ can exhibit. The minimization of $\mathrm{Tr}(W\rho)$ represents the search for the optimal entanglement witness W_{opt} subject to the constraint $W \in \mathcal{M}$. The interesting point is that by choosing different $\mathcal{M}$, E_{W} can reveal different aspects of the entanglement geometry and thus quantify entanglement under several points of view. As a matter of fact, if in the minimization procedure in (8), it is chosen to search among witnesses W such that $W \leqslant I$ (I is the identity matrix), E_{W} is nothing more than the *generalized robustness* [26], an entanglement quantifier with a rich geometrical interpretation [27, 28]. Other choices of $\mathcal{M}$ would reach other known entanglement quantifiers [25]. Moreover it is easy to see that, regardless these choices, E_{W} is a bilinear function of the matrix elements of ρ and of W_{opt}. So singularities in ρ or in W_{opt} cause singularities in $E_{\mathrm{W}}(\rho)$.

At this moment, we can follow Wu *et al* [6] and state that, if some singularity occurring in E_{W} is not caused by some artificial occurrences of non-analyticity (e.g., maximizations or some other mathematical manipulations in the expression for E_{W}—see conditions (a)–(c) in theorem 1 of [6]), then a singularity in E_{W} is both necessary and sufficient to signal a PT. It is important to note that the concept of PT considered by the authors is not thermal equilibrium PT: the PT's discussed by them are those linked with non-analyticities in the derivatives of the ground state energy with respect to some parameters as a coupling constant, i.e., quantum PTs [29]. On the other hand, it is also important to highlight that our result implies a multipartite version

of theirs. Moreover, the use of E_W to study quantum PTs can result in a possible connection between critical phenomena and quantum information processing, as E_W (via the robustness of entanglement) is linked to the usefulness of a state to teleportation processes [30, 31].

We can go further and extrapolate the concept of a PT by studying the cases where E_W presents a singularity. An interesting case is when a discontinuity happens in W_{opt} and not in ρ. This can happen for example if the set S_k presents a sharp shape (see figure 4), a situation in which occurs the recently introduced *geometric PT* [27], where the PT is due to the geometry of S_k. Besides the interesting fact that a new kind of quantum phase transition can occur, the geometric PT could be used to study the entanglement geometry. This can be made by smoothly changing some density matrix and establishing whether E_W reveals some singularity. Furthermore, E_W can be experimentally evaluated, as witness operators are linked with measurement processes [32, 33] and has been used to confirm entanglement experimentally [34]. So, the geometry behind entanglement can even be tested experimentally. A more detailed study of this issue is given in [27].

4. Conclusion and discussion

Summarizing, we have shown that entangled thermal-equilibrium systems naturally present an entanglement crossover when heated. However different entanglement quantifiers lead with this crossover differently, in the sense that, depending on the chosen quantifier this crossover is smooth or not. This implies that, when using entanglement to confirm PTs, according to some quantifiers the PT is of first-order (e.g., the negativity and concurrence), second-order (e.g., the entanglement of formation), and even though discontinuous (e.g., the IM).

With these ideas in mind it is tempting to ask some questions: Is the crossover shown here linked with some physical effect other than just vanishing quantum correlations? To be more specific, which macroscopically observed PTs have entanglement as an order parameter? From another perspective, can the way in which entanglement quantifiers lead with PTs be considered a criterion for choosing among them? Is there 'the good' quantifier to deal with such PT? Of course the patterns presented by the quantifiers depends on the mathematical definition of them. However there is not a preferable one, and one must choose the best quantifier according to each phenomenon or task. But note that entanglement is a true physical property of the system and, *a priori*, it should be possible to investigate it experimentally in each system. So, we must find practical ways to investigate the behaviour of the quantum correlations in a system before choosing how to quantify them. We hope our present contribution can motivate more research on this topic.

Finally, recent discussions have shown that the entanglement crossover is behind important quantum phenomena such as decoherence precesses [35] and entanglement transfer [36]. So similar analysis can also be performed in different contexts other than increasing temperature.

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