Holographic Photosynthesis

Irina Aref’eva and Igor Volovich

Steklov Mathematical Institute, Russian Academy of Sciences,
Gubkina str. 8, 119991, Moscow, Russia

E-mail: arefeva@mi.ras.ru, volovich@mi.ras.ru

Abstract: There are successful applications of the holographic AdS/CFT correspondence to high energy and condensed matter physics. We apply the holographic approach to photosynthesis that is an important example of nontrivial quantum phenomena relevant for life which is being studied in the emerging field of quantum biology. Light harvesting complexes of photosynthetic organisms are many-body quantum systems, in which quantum coherence has recently been experimentally shown to survive for relatively long time scales even at the physiological temperature despite the decohering effects of their environments.

We use the holographic approach to evaluate the time dependence of entanglement entropy and quantum mutual information in the Fenna-Matthews-Olson (FMO) protein-pigment complex in green sulfur bacteria during the transfer of an excitation from a chlorosome antenna to a reaction center. It is demonstrated that the time evolution of the mutual information simulating the Lindblad master equation in some cases can be obtained by means of a dual gravity describing black hole formation in the AdS-Vaidya spacetime. The wake up and scrambling times for various partitions of the FMO complex are discussed.

Keywords: holography, AdS/CFT correspondence, photosynthesis, light-harvesting complex, black holes, entanglement entropy, mutual information
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1 Introduction

The anti-de Sitter - conformal field theory (AdS/CFT) correspondence [1] and more general
holographic gravity/gauge duality play an important role in modern theoretical physics.
They have been used for description of strong interacting equilibrium and non-equilibrium
systems in high energy physics, in particular, to describe heavy-ion collisions and formation
of quark-gluon plasma [2–4], as well as in condensed matter physics [5, 6].

According to the holographic correspondence the quantum gravity (string theory) on
anti-de Sitter spacetime (AdS) is equivalent to a certain quantum field theory on the AdS
boundary. The holographic approach provides a powerful method for studying strongly
coupled quantum field theories by means of the dual classical gravitational theory in the
AdS space which is more tractable.

In last years, there has been a growing interest to study the entanglement entropy
and quantum mutual information for various quantum systems by using the holographic
approach [7]-[31] and refs therein. The entanglement entropy of a boundary region is
determined by the area of the minimal bulk surface that coincides with the entangling
surface at the boundary [7–9].

In this paper we apply the holographic approach to photosynthesis. Light harvesting
complexes (LHC) in bacteria and plants are important examples of nontrivial quantum
phenomena relevant for life which are being studied in the emerging field of quantum biol-
ology. Recent investigations of quantum effects in biology include also the process of vision,
the olfactory sense, the magnetic orientation of migrant birds as well as photon antibunch-
ing in proteins, the quantum delocalization of biodyes in matter-wave interferometry and
quantum tunneling in biomolecules, see for instance [32–37].

Photosynthesis is vital for life on Earth [38]. Photosynthesis changes the energy from
the sun into chemical energy and splits water to liberate oxygen and convert carbon dioxide
into organic compounds, especially sugars. Nearly all life either depends on it directly as
a source of energy, or indirectly as the ultimate source of the energy in their food.

Light-harvesting complexes in plants and photosynthetic bacteria include protein scaf-
folds into which pigment molecules are embedded, e.g. chlorophyll or bacteriochlorophyll
molecules. The pigment molecules absorb light and the resulting electronic excitation,
exciton, is transported between the pigment molecules until it reaches a reaction center
complex, where its energy is converted into separated charges. The process whereby the
light energy is transported through the cell is extremely efficient – higher than any artificial
energy transport process.

One models many photosynthetic light harvesting complexes by a general three-part
structure comprising the antenna, the transfer network, and the reaction center. The an-
tenna captures photons from sunlight and subsequently excites the electrons of the pigment
from their ground state. The excited electrons, which combine with holes to make excitons,
travel from the antenna through an intermediate protein exciton transfer complex to the
reaction center where they participate in the chemical reaction that generates oxygen.

Quantum coherences have been observed in two-dimensional spectroscopic studies of
energy transfer within several different light harvesting complexes. The simplest light
harvesting complex is the Fenna-Matthews-Olson (FMO) protein-pigment complex in green sulfur bacteria. We demonstrate that some numerical results on the time evolution of the mutual information for the FMO complex [39] can be obtained by using the holographic approach.

Experiments with the FMO complex have shown the presence of quantum beats between excitonic levels at both cryogenic (77°K) and ambient (300°K) temperatures [40–43]. Quantum coherence has also been seen in light harvesting antenna complexes of green plants [44] and marine algae [45]. There are also studies of quantum coherence within the reaction center [46].

Theoretical studies of excitation dynamics in the FMO complex in the single excitation subspace have demonstrated the presence of long-lived, multipartite entanglement. A study of the temporal duration of entanglement in the FMO complex using a simulation of excitation energy transfer dynamics under conditions that approximate the real environment was performed in [47]-[52]. Entanglement within the Markovian description of the FMO complex has been considered in [48, 51]. The time evolution of the mutual information in the FMO complex was studied in [50] by using simulation of the Gorini-Kossakowski-Sudarshan-Lindblad master equation. Quantum nonlocality as a function of time is studied in [53].

The paper is organized as follows.

In Sect.2 has an introductory character. Here we remind the main objects and tools of our study of the FMO complex. In Sect.2.1 has an introductory character. Here we briefly describe the FMO complex and write down the corresponding master equation. In Sect.2.1.3 the standard consideration of LHC as quantum system and entropy of entanglement and mutual information for the FMO complex are sketched. In Sect.2.1.4 we list different reductions of the FMO complex used in modern theoretical studies. In Sect.2.2 definitions of holographic entanglement entropy and mutual information, as well as the basic formula that we use in the main text are presented. In Sect.2.3 two iterative procedures to calculate the holographic entanglement entropy \( S(A_1 \cup A_2 \cup \ldots \cup A_n) \) are presented. The fist one takes into account contributions only of primitive diagrams and the second one incorporates also Boltzmann rainbow diagrams. In Sect.2.4 we remind the phase structure of the holographic mutual information \( I(A, B) \) for two belts in the static backgrounds, empty AdS\(_{d+1}\) and AdS\(_{d+1}\) black brane.

Sect.3 is devoted to the study of the time evolution of holographic mutual information for the simplest reduction of the FMO complex. We start, Sect.3.1, by calculation of holographic entanglement entropy for two site system during a quench at nonzero temperature. Then in Sect.3.2 we study holographic mutual information for two site system at nonzero temperature. In Sect.3.3 we compare the results of our calculations with the mutual information \( I(A, B) \) calculated for the reduced FMO system in [50]. In Sect.3.4 we discuss the dependencies of wake up time and scrambling times on the geometrical parameters and the initial temperature.

In Sect.4 we consider the holographic mutual information for the reduction of the FMO complex with one composite part. For this purpose in Sect.4.1 we study the phase structure of holographic entanglement entropy \( S(A \cup B \cup C) \) for the Vaidya shell in the AdS\(_d\) black
brane background. In Sect.4.2 the mutual information for 3 segments and scrambling time for this background is calculated and in Sect.4.3 we make a fit of time dependence of the mutual information at the physiological temperature ($300^\circ K$) calculated in [50] for one mixed state by the time dependence of the holographic mutual information $I(A_1 \cup A_6, A_3)$ under the global quench by the Vaidya shell in AdS$_4$.

2 Setup

2.1 FMO complex

2.1.1 Seven bacteriochlorophylls

The FMO protein complex [39] is the main light-harvesting component of the green sulfur bacteria Prosthecochloris aestuarii. It is a trimer, consisting of three identical molecular sub-units, Fig.1A. Each of the sub-units is a network of seven\(^1\) interconnected bacteriochlorophylls \{1, 2, \ldots, 7\} arranged in two weakly connected branches that are separately connected to the antenna (bacteriochlorophyll sites one and six) and jointly connected to the reaction center via site three, Fig.1B.

The theoretical models in the literature [48–51] study the dynamics of one sub-unit of the trimer. The total Hamiltonian of the system includes the non-relativistic QED Hamiltonian in the dipole approximation, phonon Hamiltonian and other environmental fields, for a derivation of the master equation in the weak coupling stochastic limit see [55] and also [56, 57].

We consider one sub-unit of the trimer which consists of seven bacteriochlorophyll sites \{1, 2, \ldots, 7\} transferring energetic excitations from a photon-receiving antenna to a reaction center, see Fig.1.

\(^{1}\)Recently, an additional bacteriochlorophyll (the eighth) pigment was discovered in each subunit of this trimer[54].
2.1.2 Master equation

We consider the nine-state model [49, 50] for excitation transfer in the single excitation approximation which is described by a 9-dimensional subspace in the Hilbert space \((\mathbb{C}^2)^\otimes 8\). The possible states for the exciton will be expressed in the site basis \(\{ |m\rangle \}_{m=1}^{7} \) where the state \( |m\rangle \) indicates that the excitation is present at site \( m \). There are also a ground state \( |G\rangle \) corresponding to the loss or recombination of the excitation and a sink state \( |S\rangle \) corresponding to the trapping of the exciton at the reaction center (there is a discussion of the “local” and “global” bases in theory of open quantum systems in [58]). The density operator for this quantum system has the following representation in the site basis:

\[
\rho = \sum_{m,n \in \{G,1,...,7,S\}} \rho_{m,n} |m\rangle \langle n | \tag{2.1}
\]

It is assumed that the density matrix satisfies the GKS-Lindblad master equation of the following form

\[
\frac{d}{dt} \rho = -i[H, \rho] + \mathcal{L}(\rho) \tag{2.2}
\]

Here the Hamiltonian \( H \) describes the coupling between the seven sites states \( |1\rangle,...,|7\rangle \):

\[
H = \sum_{m} E_{m} |m\rangle \langle m | + \sum_{m<n} V_{mn} (|m\rangle \langle n | + |n\rangle \langle m |), \tag{2.3}
\]

where \( E_{m} \) is the energy of the site \( m \) and \( V_{mn} \) describes the coupling between sites \( m \) and \( n \). A Lindblad superoperator \( \mathcal{L}(\rho) \) has the general form

\[
\mathcal{L}(\rho) = \sum_{m} \gamma_{m} (2L_{m}\rho L_{m}^{\dagger} - \{ L_{m}^{\dagger}L_{m}, \rho \}), \tag{2.4}
\]

where \( L_{m} \) are arbitrary operators and \( \gamma_{m} \) are positive constants, see for example [34]. In our case for the FMO complex the Lindblad superoperator is taken in the form [47–50]

\[
\mathcal{L}(\rho) = \mathcal{L}_{\text{diss}}(\rho) + \mathcal{L}_{\text{deph}}(\rho) + \mathcal{L}_{\text{sink}}(\rho) \tag{2.5}
\]

Here the first term \( \mathcal{L}_{\text{diss}}(\rho) \) describes the dissipative recombination of the exciton,

\[
\mathcal{L}_{\text{diss}}(\rho) = \sum_{m} \Gamma_{m} (2|G\rangle \langle m | \rho | m\rangle \langle G | - \{ |m\rangle \langle m |, \rho \}) \tag{2.6}
\]

where \( \Gamma_{m} \) is the rate of the recombination at site \( m \).

The second Lindblad superoperator \( \mathcal{L}_{\text{deph}}(\rho) \) accounts for the dephasing interaction with the environment,

\[
\mathcal{L}_{\text{deph}}(\rho) = \sum_{m} \lambda_{m} (2|m\rangle \langle m | \rho | m\rangle \langle m | - \{ |m\rangle \langle m |, \rho \}) \tag{2.7}
\]

where \( \lambda_{m} \) is the rate of dephasing at site \( m \).

The final term \( \mathcal{L}_{\text{sink}}(\rho) \) accounts for the trapping of the exciton in the reaction center:

\[
\mathcal{L}_{\text{sink}}(\rho) = \Gamma_{\text{sink}} (2|S\rangle \langle 3 | \rho | 3\rangle \langle S | - \{ |3\rangle \langle 3 |, \rho \}) \tag{2.8}
\]

It is supposed that the initial state of the FMO complex is a pure excitation at site one or site six, or a mixture of these two states.
2.1.3 Entropy of entanglement and mutual information

Let two parties $A$ and $B$ share a quantum state $\rho_{AB}$ in a Hilbert space $H_A \otimes H_B$. The von Neumann entropy of this state is

$$S(AB) = -\text{tr}(\rho_{AB} \log \rho_{AB})$$

(2.9)

Similarly, one can define the entanglement entropies

$$S(A) = -\text{tr}(\rho_A \log \rho_A), \quad S(B) = -\text{tr}(\rho_B \log \rho_B),$$

(2.10)

where the reduced density matrices $\rho_A = \text{tr}_B \rho_{AB}$ and $\rho_B = \text{tr}_A \rho_{AB}$.

The quantum mutual information $I(A; B)$ measures the correlations shared between the two parties,

$$I(A; B) = S(A) + S(B) - S(AB).$$

(2.11)

This can be written as a relative entropy and is therefore non-negative:

$$I(A; B) = S(\rho_{AB} \| \rho_A \otimes \rho_B) \geq 0$$

(2.12)

where

$$S(\rho \| \sigma) = \text{Tr}(\rho \log \rho) - \text{Tr}(\rho \log \sigma),$$

see for example [34].

Several simulations of the quantum mutual information as a function of time at cryogenic ($77^\circ K$) and physiological ($300^\circ K$) temperatures were conducted in [50]. In particular the simulations calculate the quantum mutual information with respect to several "bipartite cuts" of the sites in the FMO complex. The different cases are as follows, (Figs.1-6 in [50]):

1. The first cut was picked up where system $A$ consists of site three and system $B$ consists of sites one and six, (Figs.1 and 2 in [50]). Remind that the initial state of the complex is at site one, six, or the mixture, and the FMO complex transfers the excitation from these initial sites to site three.

2. The next bipartite cut is with the $A$ system consisting of sites one and two and the $B$ system consisting of site three, (Figs.3 and 4 in [50]).

3. Finally, the third cut was the cut where system $A$ consists of site three and system $B$ consists of all other sites, (Figs.5 and 6 in [50]). The quantum mutual information for this case should be larger than for the case of the other cuts.

2.1.4 Reductions of the FMO complex

We start from Fig.1. Several reductions of this system to more simple ones are considered. Some of them are schematically presented in Fig.2–Fig.4.
2.2 Holographic entanglement entropy

2.2.1 Static AdS background

Consider a quantum field theory on a $d$-dimensional manifold $\mathbb{R} \times \mathbb{R}^{d-1}$, where $\mathbb{R}$ and $\mathbb{R}^{d-1}$ denote the time axis and the $(d-1)$-dimensional space-like manifold, respectively. Let be given a $(d-1)$-dimensional submanifold $A \subset \mathbb{R}^{d-1}$ at fixed time $t = t_0$ and let $\partial A$ be its boundary. Then the formula for the holographic entanglement entropy $S_A$ in a CFT on $\mathbb{R} \times \mathbb{R}^{d-1}$ reads [7]

$$S_A = \frac{A(\gamma_A)}{4G_N^{(d+1)}} ,$$

(2.13)
where $A(\gamma_A)$ is the area of $\gamma_A$, that is the $d - 1$ dimensional static minimal surface in AdS$_{d+1}$ with metric

$$ds^2 = \frac{R^2}{z^2} \left( dz^2 - dt^2 + \sum_{i=1}^{d-1} dx_i^2 \right),$$

(2.14)

whose boundary is given by $\partial A$, and $G_N^{(d+1)}$ is the $d + 1$ dimensional Newton constant, $R$ is the radius of AdS$_{d+1}$.

The simplest example for the shape of $A$ is a straight belt at the boundary $z = 0$, see Fig.5,

$$A = \{x_i|x_1 \in [-l,l], x_{2,3,...,d-1} \in (-\infty, \infty)\},$$

(2.15)

![Figure 5](image_url)

**Figure 5.** The standard holographic picture of a strip configuration in three spacetime dimensions at a constant time slice. $\ell$ is the width of the belt and $D \gg \ell$. The bulk surface extended in the direction $z$ ends on the entanglement surface $A$.

In this case the area of the minimal surface, divided on the suitable constants, is [7]

$$\frac{A_{\text{vac,reg}}}{R^{d-1}D^{d-2}} = \left( \frac{1}{(d - 2)\epsilon^{d-2}} - \frac{c_0}{\epsilon^{d-2}} \right), \quad d > 2,$$

(2.16)

where $D$ is the length of $A$ in the traversal $x_{2,3,...,d-1}$-direction, $\epsilon > 0$ is the UV regularization, $c_0$ is a positive constant depending on $d$. The first term is divergent when $\epsilon \to 0$, but for our purpose it will not play a role, since we will consider the differences of entanglement entropies.

For an excited state whose gravitational dual is provided by the black brane solution with mass $m$ and the Hawking temperature $T_H = dm^{1/d}/4\pi$ (here we assume $R = 1$)

$$ds^2 = \frac{1}{z^2} \left( -f(z)dt^2 + \frac{dz^2}{f(z)} + \sum_{i=1}^{d-1} dx_i^2 \right), \quad f(z) = 1 - mz^d,$$

(2.17)

in general, it is not possible to find an explicit expression for the entanglement entropy for $d > 3$. It can be found from the integral equation relating the entropy to an auxiliary
The entanglement entropy is given by the extremum of the functional [14, 17]
\[
\frac{A}{2R^{d-1}D^{d-2}} = \int_0^\ell dx \frac{dz}{z^{d-1}} \sqrt{1 - \left[1 - m(v)z^d\right](v')^2 - 2v'z'},
\]
(2.23)
where \(z = z(x), v = v(x)\) and \(v' = dv/dx\).

The Euler-Lagrange equations corresponding to the action (2.23) read
\[
\left[1 - m(v)z^d\right]v'' + z'' - \frac{\partial_v m(v)}{2} z^d(v')^2 - d m(v)z^{d-1}z'v' = 0,
\]
(2.24)
\[
z v'' - \frac{d-2}{2} m(v)z^d(v')^2 + (d-1)[(v')^2 + 2v'z' - 1] = 0.
\]
(2.25)
For the system of equations (2.24), (2.25) we will solve numerically the Cauchy problem with initial data (2.27), (2.27)

\[ z(0) = z_*, \quad v(0) = v_*, \]  
\[ z'(0) = v'(0) = 0, \]  

We are interested in finding solutions that reach the boundary at some point, that we identify with \( \ell \) in (2.23) at the boundary time \( t \):

\[ z(\ell) = 0, \quad v(\ell) = t. \]

Equations (2.24), (2.25) have an integral of motion

\[ \left( \frac{z_*}{z} \right)^{2(d-1)} = 1 - \left[ 1 - m(v)z^d \right] (v')^2 - 2v'z'. \]  

Due to this identity the integral in (2.23) can be substantially simplified to give

\[ \frac{A_{\text{reg}}}{2R^{d-1}D^{d-2}} = \int_0^{\ell-\epsilon} \frac{z_*^{d-1}}{z^{2(d-1)}} \, dx, \]  

where we introduce regularization \( \epsilon > 0 \). This integral contains the UV divergence when \( \epsilon \to 0 \). The renormalized version of (2.30) can be written as [14, 17]

\[ \frac{A_{\text{ren}}}{2R^{d-1}D^{d-2}} = \int_0^{\ell-\epsilon} \frac{z_*^{d-1}}{z^{2(d-1)}} \, dx - \frac{1}{(d-2)(z(\ell-\epsilon))^{d-2}}, \quad d > 2, \]  

and regularization can be removed. Note, that in the case of \( d = 2 \) [14, 17]

\[ \frac{A_{\text{ren}}}{2R} = \int_0^{\ell-\epsilon} \frac{z_*}{z^2} \, dx + z_* \log(z(\ell-\epsilon)). \]  

It is quite straightforward to find the dependence of the renormalized entanglement entropy on \( z_* \) and \( v_* \). To find the dependence of the entanglement entropy on \( \ell \) and \( t \) one has to parametrize the solutions to (2.27)-(2.25), not by \( (z_*, v_*) \), but by \( \ell \) and \( t \).

It happens that the values of \( \ell \) and \( t \) are very sensitive to the initial data (2.26), and one needs a special numerical procedure to find the pair \( (z_*, v_*) \) corresponding to the given pair \( \ell, t \) with large values of \( \ell, t \), see [17, 25, 28] and refs therein for more details. It is interesting to note that the case when \( m_0 > 0 \) in (2.22) is more stable than the case \( m_0 = 0 \).

In Fig.7 the dependence of the renormalized holographic entanglement entropy on \( t \) and \( \ell \) for the propagating Vaidya shell in the four dimensional black brane background with \( f = f(z, v) \) given by (2.20) and (2.22) is presented. As compare with the dependence of the holographic entanglement entropy for the Vaidya AdS\(_4\) metric the entropy does not go to fixed value for large \( \ell \), but as both go to constant values for large times. The same is shown in Fig.8 for the three dimensional black brane background.

Note that the similar technique has been intensively used in study the thermalization processes, especially for non-conformal invariant backgrounds, see [25, 28, 60–62] and refs therein.

\(^2\)In our calculation the width of the belt is \( 2\ell \), although on some pictures we omit the factor 2.
Figure 6. The time dependence of the holographic entanglement entropy $A_{\text{ren}}(\ell,t)$, after the corresponding initial state subtraction, for the Vaidya metric in the four dimensional black brane background with $f = f(z,v)$ ($m_0 = 0.25$, $m = 1$ in the left panel and $m_0 = 0$, $m = 1$ in the right panel) at fixed $\ell = 1,1.5,2,2.5,3,3.5$ (gray, blue, darker cyan, green, purple and magenta, respectively). For all cases $\alpha = 0.2$.

Figure 7. The renormalized holographic entanglement entropy $A_{\text{ren}}(\ell,t)$, up to the normalizing factor, for the Vaidya metric in the four dimensional black brane background with $f = f(z,v)$ ($m_0 = 0.25$, $m = 1$ in the left panel and $m_0 = 0$, $m = 1$ in the right panel) at fixed $t = 0,1,2,3,4$ (blue, orange, green, red and darker blue, respectively) as function of $\ell$. For all cases $\alpha = 0.2$.

2.3 Iterative procedure to calculate $S(A_1 \cup A_2 \cup \ldots \cup A_n)$

In this section we present the rules that help to calculate the holographic entropy for $n$ disjoint objects. Here we consider for illustration a particular case of $n$-segments. This problem has been studied in several papers [15–17, 22, 23, 31]. It is substantially simplified in the case of equal length strips and equal separation between them. However in order to deal with holographic description of the FMO complex, we have to find the entropy for non-equal length strips.

To find the entropy one has to find the global minimum among all possible configurations. To specify all possible configurations corresponding to local minimum surfaces it is convenient to use the diagrammatic language. In special cases, it happens that only primitive diagrams contribute to the entropy. The primitive diagrams are diagrams that do not contain cross-sections of the connected lines and also do not contain diagrams with
"engulfed" sub-diagrams in the terminology used in [23]. Note that the class of primitive diagrams contains less diagram then so-called rainbow diagrams in the Boltzmann quantum field theory [63]. It is possible that for more complicated backgrounds one has to take into account more diagrams then only the primitive diagrams.

\[
\begin{align*}
  & (A \cup B \cup C)_p \\
  = & \\
  & (A, B, C)_{c, \text{non-cr}} \\
  = & \\
  & (A) || (B) C_c \\
  & (A) || (B) || (C) \\
  & (A B)_c || (C) \\
  & (A, B)_{c, \text{non-cr}} \\
  = & \\
  & (A) || (B)
\end{align*}
\]

**Figure 9.** The decompositions (2.35) for 3 and 2 segments that include only primitive diagrams. Selections of primitive diagrams are indicated by dashed lines.

In Fig.9 we show primitive diagrams that contribute to calculation of the entanglement entropy for 2 and 3 segments. There are three competing minimal surfaces for 2 segments A and B, see Fig.17 below, one surface corresponds to a "disjoint" configuration \((A||B)\), the second to a "connected non-crossing" one \((A, B)_{c, \text{non-cr}}\), the third to a "crossing" one.
\((A, B)_{c, cr}\), and we can write the symbolic representation
\[
(A \cup B) = (A)\|\| (B) + (A, B)_{c, non-cr} + (A, B)_{c, cr},
\]  \hspace{1cm} (2.33)

here the brackets in \((A \cup B)\) mean that we deal with corresponding diagrams and in the RHS of (2.33) we list these diagrams. Due to a possible change of the leader in this competition the system may undergo a phase transition under change the geometrical parameters, see [22, 23].

For 3 segments one can write the full decomposition as
\[
(A \cup B \cup C) = (A)\|\| (B)\|\| (C) + (A, B, C)_{c, cr} \hspace{1cm} (2.34)
\]
\[+(A, B, C)_{c, non-cr} + (A, B)_{c} ||| (C) + (A)\|\| (B, C)_{c} + (A, B)_{c} ||| (C)\]

The first term represents the totally disconnected diagram (the disconnected parts are separated by symbol \(||\)). The second and the third terms represent the crossing (“intersecting”) and non-crossing connected diagrams. The last three terms correspond to diagrams with disjoint parts, wherein the last term corresponds to the rainbow diagram. The rainbow diagram contains an “engulfed” subdiagram (in terminology used in [23]), that is indicated by writing the corresponding symbol by the bold letter B and the curl underbrace bracket.

We call the diagram corresponding to the first, third, fourth and fifth terms as primitive diagrams. We use the same terminology also for \(n\)-segment cases. Due to the competition between different terms in decomposition (2.34) there are phase transitions. The number of possible phases depends on number of diagrams that contribute to the entropy. For 3 segments of equal length and with unequal separations, the competition between primitive diagrams gives rise to, generally speaking, 4 phases [15–17, 22, 23]. The similar situation takes place for non-equal lengths and in Fig. 10 we present the phase diagrams for \(l_1 \neq l_2 \neq l_3\) and equal separations.

To calculate \(S(A_1 \cup A_2 \cup ... \cup A_n)\) taking into account only the primitive diagrams we use the following representation
\[
(A_1 \cup A_2 \cup ... \cup A_n)_p = (A_1, A_2, ...A_n)_c + \sum_{j=1}^{n-1} (A_1, A_2, ...A_j)_c \ast (A_{j+1} \cup A_2 \cup ... \cup A_n)_p \hspace{1cm} (2.35)
\]

where \((A_1, A_2, ...A_j)_c\) is the bulk connected surface ending on segments \(A_1, A_2, ...A_n\) constructed without any crossing lines. There is only one such surface for a given number of segments. In (2.35) there is the symbol \(\ast\) that means that sub-diagrams on the left and on the right of the symbol compose the same \(n\)-segment diagram. We will omit this symbol in what follows. The decomposition (2.35) for 3 and 7 segments is shown in Fig. 9 and Fig. 12, respectively (or the moment, the reader can ignore the different colors for segments and connecting lines in Fig.12). In these pictures contributions to \((A_1 \cup A_2 \cup ... \cup A_n)_p\) are shown by the enveloping rectangles.
Figure 10. A. The phase diagrams for 2 strips, $A, B$ with unequal lengths $l_1, l_2$. The green color regions correspond to the bulk surface $(A) || (B)$, the cyan color regions correspond to the bulk surface $(A, B)_c$. B. The phase diagrams for 3 strips, $A, B, C$, with unequal lengths $l_1, l_2, l_3$. The green color regions correspond to the bulk surface $(A) || (B) || (C)$, the blue color regions correspond to the bulk surface $(A B)_c || (C)$ and the cyan color corresponds to the bulk surface $(A, B, C)_c, \text{non-cr}$. Different colors regions are separated by the curves that are the transition lines. In the left plot $l_1 = l_2$, in the middle plot $l_2 = 0.3l_1$ and in the right plot $l_2 = 3l_1$ and we vary $l_1$ and $l_2$ keeping the distances between segments fixed. All plots correspond to AdS$_4$.

Figure 11. The phase diagrams for 4 strips, $A_1, A_2, A_3, A_4$ with unequal lengths $l_1, l_2, l_3, l_4$. The gray color regions correspond to the bulk surface $(A_1) || (A_2) || (A_3) || (A_4)$, the green color regions correspond to the bulk surface $(A_1, A_2, A_3, A_4)_{\text{non-cr}}$, the cyan color regions correspond to the bulk surface $(A_1) || (A_2 A_3 A_4)_c$ and the purple color corresponds to the bulk surface $(A_1 A_2 A_3 A_4)_c || (A_4)$. Dark green and dark blue regions correspond to the bulk surface $(A_1)(A_2) || (A_3 A_4)_c$ and $(A_1, A_2)_c || (A_3)(A_4)$, respectively. Different colors regions are separated by the curves that are the transition lines. In the left plot $l_1 = l_2$, $l_3 = l_4$, in the middle plot $l_2 = 0.5l_1$, $l_4 = 0.5l_3$ and in the right plot $l_2 = 1.5l_1$, $l_4 = 1.5l_3$ and we vary $l_1$ and $l_2$ keeping the distances between segments fixed. All plots correspond to AdS$_4$.

To calculate $S(A_1 \cup A_2 \cup \ldots \cup A_n)$ taking into account also the Boltzmann rainbow diagrams one can use the following representation

$$(A_1 \cup A_2 \cup \ldots \cup A_n)_B = (A_1, A_2, \ldots A_n)_{\text{cw-B}} + \sum_{j=1}^{n-1} (A_1, A_2, \ldots A_j)_{\text{cw-B}} \ast (A_{j+1} \cup A_2 \cup \ldots \cup A_n)_B$$

(2.36)
Figure 12. Recursive procedure (2.35) to calculate \((A_5 \cup A_6 \cup A_7 \cup A_1 \cup A_2)_p\)

where \((A_1, A_2, ... A_n)_{cwB}\) are connected diagrams with Boltzmann insertions,

\[
(A_1, A_2, ... A_j)_{cwB} = \sum_{\{i_q, k_q\}} \left( A_1, ... A_i_1, \left( A_{i_1+1} \cup A_{i_1+2} \cup ... A_{i_1+k_1} \right)_B A_{i_1+k_1+1}, ... \right)
\]

Here the Boltzmann insertions are indicated by the bold letters and curl underbrace brackets. Note, that \(cwB\) diagrams are not connected, but if we remove the Boltzmann insertions we are left with the connected diagrams. In particular, if we remove the Boltzmann insertions in the RHS of (2.37) we left with connected diagrams

\[
(A_1, ... A_i_1, A_{i_1+k_1+1}, ... A_{i_1+i_2+k_1+1}, A_{i_1+i_2+k_1+2}, ... A_{i_1+i_2+k_1+k_2})_c
\]

Comparing (2.35) with (2.36) and (2.37) we see that the Boltzmann diagrams are composed by insertions of low order Boltzmann diagrams to primitive diagrams.
Figure 13. The decomposition (2.37) for 3 segments. Selections of Boltzmann diagrams are indicated by double dashed lines. There are no difference between the primitive and the Boltzmann selections for two segments, but there is the difference for 3 and more segments.

2.4 Holographic mutual information

The mutual information $I(A;B)$ of two entangling regions $A$ and $B$ is defined by (2.11):

$$I(A;B) = S(A) + S(B) - S(A \cup B), \quad (2.38)$$

where $S(A \cup B)$ is the entropy of the union of two regions. Holographic definition of the mutual information $I(A;B)$ just means that we calculate all terms in the RHS of (2.39) holographically.

To find $S(A \cup B)$ one has to find the minimal surface between two competing ones, "joint" and "disjoint" surfaces, as shown in Fig.17. The winner, in the case of vacuum background, depends only on the ratios of segments to the distance between them. It is obvious that $I(A;B)$ is equal to zero for the case when the minimal surface is realized on the "disjoint" configuration. Generally speaking, $I(A,B)$ undergoes a first order phase transition as one increases the distance between two strips [9, 11, 19]

$$I(A;B) = \begin{cases} I(A;B), & \text{if } I(A;B) \geq 0 \\ 0, & \text{if } I(A;B) \leq 0 \end{cases} \quad (2.39)$$

$$I(A;B) \equiv S(A) + S(B) - S(A + x + B) - S(x), \quad (2.40)$$

where $S(A)$ are areas of surfaces entangling the belt (stript) with segment $A$. In the case of the AdS$_d$ background $I(A;B)$ is given by

$$\frac{I(A;B)_{\text{vac}}}{2L^{d-2}c_0} = -\frac{1}{\ell^d} - \frac{1}{\ell_1^{d-2}} + \frac{1}{(\ell_1 + \ell_2 + x)^{d-2}} + \frac{1}{x^{d-2}}, \quad (2.41)$$
here $d > 2$. The region where the mutual information is nonzero depends on the ratios of parameters $\ell_1/x, \ell_2/x$ in the case of $AdS_d$, and on the ratios of parameters $\ell_1/x, \ell_2/x$ and $z_h/x, z_h = m^{-1/d}$, in the case of AdS$_d$ black brane, see 14 and Fig.15. From these plots we clearly see that the mutual information of two static belts is maximal when the system is in the vacuum state.

![Figure 14](image1.png)

**Figure 14.** The regions of non-zero holographic mutual information for two strips with the widths $\ell$ and $L$ and distance $x$ for two thermal states whose gravity duals are given by the AdS$_4$ black brane metric (2.17) with $m = 0.25$ and $m = 1$. The region corresponding to $m = 1$ is inside the region corresponding to $m = 0.25$.

![Figure 15](image2.png)

**Figure 15.** The density plots of the holographic mutual information for two strips with the widths $\ell_1$ and $\ell_2$ and fixed distance $x = 0.08$ for the static vacuum state whose gravity dual is the AdS$_4$ metric (the left plot) and two thermal states whose gravity duals are provided by the AdS$_4$ black brane metric (2.17) with $m = 0.25$ and $m = 1$, respectively (the middle and the right plots).

### 3 Holographic studies of simplest FMO complex

#### 3.1 Holographic entanglement entropy for two site system during a quench at nonzero temperature.

As has been mention in Sect.2.1.4, the simplest model of LHC is the two systems model. We can consider two parallel infinite strips with non-equal widths $2\ell_1$ and $2\ell_2$ separated by...
a distance $2x$ in a $d$-dimensional field theory as depicted in Fig.16 as a simplest model of LHC and find the mutual information induced by the coming photon. This coming photon we model by the Vaidya shell.

The holographic mutual information for two parallel strips in static backgrounds and in the Vaidya AdS has been studied in several papers [10, 15–17, 22, 30]. In particular for equal widths of segment in certain limits the analytical results have been obtained [22]. The specificity of our consideration here is that we want to consider the time dependence of the mutual information during a global quench of a medium that already has high temperature. The corresponding holographical model is given by the Vaidya shell propagating in the AdS$_{d+1}$ black brane background. We also compare the obtained time dependence with the time dependence of the thermalization process started from the zero temperature.

![Schematic picture of locations of the excited complex (A) and the out site (B), that sends the information to the reaction center, and the infalling photon.](image)

**Figure 16.** Schematic picture of locations of the excited complex (A) and the out site (B), that sends the information to the reaction center, and the infalling photon.

As already has been mentioned in Sect.2.3, equation 2.33, given the two disconnected regions $A$ and $B$ in the boundary, there are three configurations of hypersurfaces extending in the bulk whose boundaries coincide with $\partial(A \cup B) = \partial A \cup \partial B$: the "disjoint" configuration, the “connected” configuration, given by a bridge connecting $A$ and $B$ through the bulk and the "crossing" configuration, that looks as a configuration with cross-sections in the projection on the $(x, z)$-plane, Fig.17. The "crossing" configurations do not contribute to the holographic entropy calculations [22, 23], in the static AdS and AdS black brane backgrounds. They also do not contribute to the same calculations during the thermalization process described by the Vaidya AdS metric [17]. We have checked numerically that they do not contribute in the case of the Vaidya AdS black brane metric during the transition from the black brane with mass $m_0$ to the black brane with mass $m_0 + m$, see cartoon plots in Fig.18. In these plots we show the leading contributions to the entangle-
Figure 17. Illustration of bulk surfaces anchored to the boundaries of disjoint regions A and B. The surfaces started and ended on the boundaries of the same region are shown by the same color as the region, meanwhile the surfaces connecting the ends of different regions are shown by blue lines. In the case of considered here holographic models we do not obligate to take into account the diagram with crossing lines depicted in the last line.

Figurement entropy for 2 strips, A and B, with unequal lengths $l_1, l_2$, at different times during the transition from the black brane configuration with the small mass $m_0$ to the large mass $m$ in AdS$_3$. The green color regions correspond to the bulk surface $(A)_{||}(B)$, the blue color regions correspond to the bulk surface $(B C)_c$. In our program we have used the red color to indicate contribution of the bulk surface $(A B)_{c,c}$, but we have not seen red regions for all variety of parameters $0.2 < l_1, l_2, x < 1.5, 0 < t < 4$. Transition lines separate the different color region and as usual are interpreted as the lines of topological phase transitions. Note that one can solve this problem analytically for the case of infinitely thin shell in AdS$_3$ black brane.

3.2 Holographic mutual information for two site system at nonzero temperature.

Let us first consider the holographic mutual information $S(A \cup B)$ for the Vaidya shell in the three dimensional AdS black brane background with $f = f(z, v)$ given by (2.20) and (2.22), and two segments shown in Fig.17, as function of the boundary time $t$ at fixed $l_1, l_2, x$. This quantity depends on many parameters, $l_1, l_2, x, m, m_0$ and $\alpha$ and we perform our analysis numerically. On the right in Fig.17 we show the case $m_0 = 0.25$ and on the left we show for comparison the case $m_0 = 0$ considered before in [16, 17]. The same color curves correspond to the same fixed values of $l_1$ and $x$, herewith different style lines (solid, dashed and dotted) correspond to different values of $l_2$ for both cases, $m_0 = 0.25$ and $m_0 = 0$.

We see that some color and style lines present in both, left and right plots in Fig.19, but some color and style lines present only in the left plot in Fig.19. In particular, there are no purple lines in Fig.19.B. Notice that the character of time dependences shown in the left and right plots are the same. There are curves that start from non-zero value of the mutual
Figure 18. Cartoon diagrams that show contributions of various diagrams to the entanglement entropy for 2 strips, $A$ and $B$, with unequal lengths $l_1, l_2$, at different times during the transition from the black brane configuration with the small mass $m_0$ to the large mass $m$ in $\text{AdS}_3$. The green color regions correspond to the bulk surface $(A) \parallel (B)$, the blue color regions correspond to the bulk surface $(BC)_c$, the red color regions correspond to the bulk surface $(AB)_{c,cr}$ (we do not see red regions). Different colors regions are separated by the curves that are the transition lines. In the top plots $l_2 = l_1$, and $t = 0, 1, 2, 3$, in the bottom plots $l_2 = 2l_1$, and we vary $l_1$ and $x$. All plots correspond to $\alpha = 0.2$.

Figure 19. Holographic mutual information $I(A, B)$, up to the normalizing factor, for the Vaidya metric in the three dimensional black brane background with $f = f(z, \nu)$ given by (2.20) and (2.22) ($m_0 = 0, m = 1$ for the panel $A$ and $m_0 = 0.25, m = 1$ for the panel $B$) and two segments shown in Fig.17, as function of the boundary time $t$ at fixed $l_1, l_2, x$. The same color curves are characterized by fixed values of $l_1$ and $x$ and varying $l_2$. Blue lines correspond to $l_1 = 1.5$ and $x = 0.2$ and solid, dashed and dotted styles correspond to $l_2 = 1.5, 1$ and $0.5$, respectively; green lines correspond to $l_1 = 1.5$ and $x = 0.4$ and solid, dashed and dotted styles correspond to $l_2 = 1.5, 1.2$ and $0.9$, respectively; purple lines correspond to $l_1 = 1.5$ and $x = 0.6$ and solid, dashed and dotted lines correspond to $l_2 = 1.5, 1.4, 1.3$; dark cyan lines correspond to $l_1 = 1.7$ and $x = 0.2$ and solid, dashed and dotted lines correspond to $l_2 = 1.5, 1.2, 0.9$. For all cases $\alpha = 0.2$. We see that there are no purple lines in plots B.

Information $I_0$, then increase during some time $t_{max}$ up to some maximal value, $I_{max}$ and then during the saturation time $t_s$ go to other constant value $I_s$. Increasing the starting
temperature we decrease the corresponding $t_r$ and $t_s$. There are also curves that start from $I_0 \neq 0$, reach $I_{\text{max}}$ and then at the scrambling time $t_{sc}$ become zero. At the scrambling time any sort of correlations, in particular the exchange of information, is erased. There is also the regime when the mutual information starts from zero at wake up time, $t_{wu}$, then it increases up to the maximum and when becomes zero at $t = t_{sc}$. In this regime the time dependence has the bell form and it is more interesting for us, see Sect.3.3. There are also geometrical configurations, when $I$ is zero at all times. These configurations correspond to the cases with large distances $x$.

The time dependence, in the logarithmic time scale, of the holographic mutual information $S(A \cup B)$ for the Vaidya shell in the four dimensional AdS black brane background is presented in Fig.20. Comparing Fig.20 and Fig.19 we see that the qualitative features of the curves are the same.

![Figure 20](image)

**Figure 20.** Holographic mutual information $I(A, B)$, up to the normalizing factor, for the Vaidya metric in the four dimensional black brane background with $f = f(z, v)$ given by (2.20) and (2.22) ($m_0 = 0, m = 1$ for the left panel and $m_0 = 0.25, m = 1$ for the right panel) and two belts shown in Fig.16, as function of the boundary time $t$ (in the logarithmical scale) at fixed $l_1, l_2$ and $x$. The same color curves are characterized by fixed values of $l_1$ and $x$ and varying $l_2$. For all green lines $l_1 = 1.5, x = 0.2$ and the solid, dashed and dotted green lines correspond to $l_2 = 1.5, 1.2, 0.9$, respectively; for all purple lines $l_1 = 1.5, x = 0.6$ and the solid, dashed and dotted purple lines correspond to $l_2 = 1.5, 1.4, 1.3$, respectively. For all cases $\alpha = 0.2$

3.3 Matching holographic calculations to the simulation results.

It is obvious that we find the scaling behavior of the holographic mutual information only up to normalization factors. To fit the mutual information for a given physical system there are 3 numerical parameters in our disposal: the $(d+1)$- dimensional gravity constant, the radius of the AdS and the scale, that in our case can be identified with the black brane mass. We compare the results of our calculations with the mutual information $I(A; B)$ calculated for the reduced FMO system in [50], where system A consists of site three and system B consists of site one, see Fig.3a in [50]. We reproduce this curve in Fig.21 by the purple dashed line. In Fig.4a of [50] this quantity at physiological temperature (300°K) is presented. We reproduce this curve in Fig.21 by the red dashed line. We see that in this
particular case the purple curve has a maximum approximately twice higher than the red one. As it is shown in Fig.21 these two curves fit two curves that we take from Fig.20 for particular choices of the geometry of two strips.

It is interesting to note, that the mutual information calculated in [50] for the reduced FMO system, where system A consists of site three and system B consists of site six, or two, see Fig.1b and 3b in [50], has the two-humped form. We can reproduce this form of the time dependence of the mutual information taking two thin shells Vaidya AdS \(d + 1\) metric with

\[
m(v) = \frac{m_1}{2} \left(1 + \tanh \frac{v}{\alpha}\right) + \frac{m_2}{2} \left(1 + \tanh \frac{v - v_0}{\alpha}\right),
\]

(3.1)

cf.[59].

**Figure 21.** The purple and red dashed lines show the time dependence of the mutual information of the reduced FMO system calculated in [50] at 70\(^\circ\)K and 300\(^\circ\)K temperature, respectively. The green and purple solid lines show the rescaled time dependence of the holographical mutual information presented in Fig.20 for the cases of the global quench in AdS\(_4\) and AdS\(_4\) black brane, respectively.

### 3.4 Wake up and scrambling times

As we have seen in Sect.3.2 there are configurations for which the time dependence of the mutual information has the bell form, see also plots in Fig.22. We see that for some time the mutual information is equal to zero (or very small) then at the wake up time \(t_{wu}\) it starts to increase, reaches the maximum at time \(t_{max}\) and then decreases and vanishes at the scrambling time \(t_{scr}\). This behaviour can be explained by a causality argument [16]. It is supposed that before the quench there is a finite correlation length in the system. Therefore after the quench only excitations created at nearest points will be entangled. At later times, such entangled pairs will only contribute to the mutual information between two intervals, if each interval contains one of the two particles.

The scrambling time is the time scale at which all correlations in a system have been destroyed after introducing a perturbation [30]. One defines the scrambling time as the
Figure 22. We show typical bell-like profiles of the time dependence of the mutual information for Vaidya quenches in the AdS\(_4\) (the left plot) and in the AdS black brane (the right plot).

Figure 23. A. The domains corresponding to the bell profiles of time dependence of the mutual information after the Vaidya quench in the AdS\(_4\) (the domain between green lines) and in the AdS black brane (the domain between purple lines) for equal width belts and different distances between them. B. The blue and red dashed lines show the time dependence of the mutual information of the reduced FMO system calculated in [50] at 70\(^\circ\)K and 300\(^\circ\)K temperature, respectively. The green and purple solid lines show the rescaled time dependence of the holographical mutual information for \(l_1 = 0.8, l_2 = 0.8\) and \(x = 0.5\) and \(x = 0.4\) for cases of the global quench in AdS\(_4\) and AdS\(_4\) black brane, respectively.

Numerical results show that all these time scales depend on the geometry as well as on the form of the quench. Plots in Fig.22 show that the wake up time is very sensitive to the change of distances between segments, while the scrambling time is not so sensitive. In Fig.23.A we show the domains corresponding to the bell profiles of time dependence of the mutual information after the Vaidya quench in the AdS\(_4\) (the domain between green lines) and in the AdS black brane (the domain between purple lines) for equal width belts and different distances between them. We see that the gaps where the bell profiles are available are quite narrow. The gaps corresponding to initial vacuum state and the state
with non-zero temperature are not crossing. By this reason our fitting with results [50] have been performed for different geometries. In the case of infinitely thin shell these time scales admit analytical studies [20].

4 Holographic studies of the FMO complex with one composite part

In this section we consider holographic description of the quantum mutual information for the reduction of the FMO complex with one composite part.

4.1 Phase structure of holographic entanglement entropy $S(A \cup B \cup C)$ for the Vaidya shell in the AdS$_d$ black brane background

In this section we consider the phase structure of holographic entanglement entropy $S(A \cup B \cup C)$ for the Vaidya shell in the three dimensional AdS black brane background with $f = f(z, v)$ given by (2.20) and (2.22), and 3 segments shown in Fig.17, at different times during the quench. This quantity depends on many variables, $l_1, l_2, l_3, x, y, m, m_0$ and $\alpha$, and we can perform our analysis only numerically, see Fig.24. In these plots contributions of various diagrams to the entanglement entropy for 3 strips, $A, B, C$, with unequal lengths $l_1, l_2, l_3$ at different times during the transition from the black brane configuration in AdS$_3$ with the small mass $m_0$ to the large mass $m$ are shown. We see that there are plots there the contribution to the holographic entanglement entropy is given by the ”engulfed” diagram. These regions are colored yellow in images in Fig.24. The images that contain yellow regions are located at the intersections of the second column and top and middle rows. Hence we have to take into account these diagrams in the analysis of the mutual information. To this purpose we use the diagram technique described in the end of Sect.2.3.
Figure 24. Cartoon diagrams that show the contributions of various diagrams to the entanglement entropy for 3 strips, A, B, C, with unequal lengths $l_1, l_2, l_3$ at different times during the transition from the black brane configuration with the small mass $m_0$ to the large mass $m$ in AdS$_3$. The green color regions correspond to the bulk surface $(A)\|(B)\|(C)$, the blue color regions correspond to the bulk surface $(A)\|(B\,C)_c$, the gray color regions correspond to the bulk surface $(A\,B)_c\|(C)$, the cyan color corresponds to the bulk surface $(A,B,C)_{c,\text{non-ct}}$ and the yellow regions correspond to the bulk surface $(A,B,C)_c$. Different colors regions are separated by the curves that are the transition lines. In the top plots $l_2 = l_3, x = 0.4, y = 0.4$, in the middle plots $l_2 = l_3, x = 0.2, y = 0.5$ and in the bottom plots $l_2 = 0.5\,l_1, x = 0.4, y = 0.5$ and we vary $l_1$ and $l_3$ keeping the distances between segments fixed. All plots correspond to $\alpha = 0.2$. 

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Figure 25. Cartoon diagrams that show the contributions of various diagrams to the entanglement entropy for 3 strips, $A, B, C$, with unequal lengths $l_1, l_2, l_3$ at different times during the transition from the black brane configuration with the small mass $m_0$ to the large mass $m$ in AdS$_4$. The green color regions correspond to the bulk surface $(A)||(B)||(C)$, the blue color regions correspond to the bulk surface $(A)||(B C)_c$, the gray color regions correspond to the bulk surface $(A B)_c||(C)$, the cyan color corresponds to the bulk surface $(A, B, C)_{c, non-cr}$ and the yellow regions correspond to the bulk surface $(A_n C)_c$. Different colors regions are separated by the curves that are the transition lines. In the top plots $l_2 = l_3$, $x = 0.5$, $y = 1$, in the middle plots $l_2 = 0.4l_3$, $x = 0.4$, $y = 0.5$ and in the bottom plots $l_2 = 0.5l_1$, $x = 0.5$, $y = 1$ and we vary $l_1$ and $l_3$ keeping the distances between segments fixed. All plots correspond to $\alpha = 0.2$.

4.2 Mutual information for (1,6|3)-reduction of the FMO complex and scrambling time

In the section we will consider also the mutual information for a system one part of which consists on two disjoint parts. Just this system corresponds to one of simplest reduce FMO
complexes presented in Fig. 2. Applying to this system the general definition (2.38) we get

\[ I(A \cup B;C) = S(A \cup B) + S(C) - S(A \cup B \cup C), \]  

(4.1)

where \( S(A \cup B \cup C) \) is the entanglement entropy for the union of three subsystems. \( I(A \cup B, C) \) is related with the tripartite information which is defined for a system consisting of three disjoint parts as follows

\[ I_3(A;B,C) = S(A) + S(B) + S(C) - S(A \cup B) - S(A \cup C) - S(B \cup C) + S(A \cup B \cup C). \]  

(4.2)

The tripartite information can be positive, negative or zero, however the holographic tripartite information is always negative, i.e. \( I_3(A;B,C) < 0 \). The validity of this inequality means that the holographic mutual information is monogamous [15]. The tripartite information can be written in terms of mutual information as follows

\[ I_3(A,B,C) = I(A;B) + I(A;C) - I(A;B \cup C). \]  

(4.3)

We take \( A = A_6, B = A_1, C = A_3 \), where \( A_i, i = 1, 3, 6 \) are 1, 3 and 6 sites of the \((1,6|3)\)-reduction of the FMO complex. We assume that \( A_6, A_3, A_1 \) are three strips of length \( l_1, l_2 \) and \( l_3 \), and separated by distances \( x \) and \( y \), Fig.26.

![Figure 26](image_url)

**Figure 26.** Brown segments show 6 and 1 sites location and the green one shows 3 site location for \((1,6|3)\)-reduction of the FMO complex, depicted in Fig.2.

In the notations introduced in Sect.2.3 and the geometry presented in Fig.26 we can write

\[ S((A_6, A_1)_{joint-ncr}) = S(l_1 + l_2 + l_3 + x + y, t) + S(l_2 + x + y, t) \]  

(4.4)

\[ S((A_6, A_1)_{dis}) = S(l_1, t) + S(l_3, t) \]  

(4.5)

\[ S((A_6, A_1)_{joint-cr}) = S(l_1 + l_2 + l_3 + x + y, t) + S(l_2 + l_3 + x + y, t) \]  

(4.6)

where \( S(l, t) \) is the holographic entropy given by (2.31) or (2.32).

\[ S(A_1 \cup A_6) = \min\{S((A_6, A_1)_{joint-ncr}), ((A_6, A_1)_{dis}), ((A, B)_{joint-cr})\} \]  

(4.7)
To get \( S(A_6 \cup A_3 \cup A_1) \) for three segments we have to take into account the following competing contributions

\[
S((A_6||A_3||A_1)) = S(l_1, t) + S(l_2, t) + S(l_3, t)
\]

\[
S(A_6||(A_3, A_1)_{n, r}) = S(l_1) + S(l_2 + l_3 + y, t) + S(y, t)
\]

\[
S((A_6, A_3)_{n, r}||A_1) = S(l_1 + l_2 + x, t) + S(x, t) + S(l_3, t)
\]

\[
S(A_6 \overset{3}{\longrightarrow} (A_1)_{n, r}) = S(l_1 + l_2 + l_3 + x + y, t) + S(l_2 + x + y, t) + S(l_2, t)
\]

\[
S((A_6, (A_3, A_1)_{n, r}) = S(l_1 + l_2 + l_3 + x + y, t) + S(x, t) + S(y, t)
\]

\[
S((A_6, A_3)_{n, r}||A_1) = S(l_1 + l_2 + l_3 + x + y, t) + S(l_2 + x, t) + S(l_2 + y, t)
\]

\[
S((A_6, A_3)_{n, r}||A_1) = S(l_1 + l_2 + x + y, t) + S(l_3 + y, t)
\]

\[
S((A_6, A_3)_{n, r}||A_1) = S(l_1 + x, t) + S(l_2 + l_3 + x + y, t) + S(y, t)
\]

and

\[
S(A_6 \cup A_3 \cup A_1) = \min \left\{ S((A_6||A_3||A_1)), S(A_6||(A_3, A_1)_{n, r}), S((A_6, A_3)_{n, r}||A_1), S(A_6 \overset{3}{\longrightarrow} (A_1)_{n, r}) \right\}
\]

Let us note, that for some particular background [23] and refs therein, we can ignore contribution of (4.6), (4.11), (4.14), (4.15) and (4.16).

The time dependence of the holographic mutual information \( I(A_6 \cup A_1; A_3) \) for the Vaidya metric in the four dimensional black brane background with \( f = f(z, v) \) given by (2.20) and (2.22) \((m_0 = 0.25, m = 1)\) and the \( x_1 \)-projection of the 3 belts configuration shown in Fig.26, at fixed \( l_1, l_2, l_3, x, y \) is presented in Fig.27. The lines of the same style (by the style we mean the color and the type of the line) correspond to the same \( l_1, l_2, l_3 \) and \( y \), but different values of \( x \), the distance between the sites ”3” and ”1” of the FMO complex presented in Fig.2. Fig.28 and Fig. 29 show different plots collected in Fig.27.

We observe that the evolution of the holographic mutual information for the case when one part of the system is consisting from two disjoints subsystems, globally resembles the case of two simple parts, but locally there are some changes. More specifically, as in the case of two simple parts, see Sec.3.2, globally there are 4 different behaviors: the mutual information is 0 at all times; the mutual information starts from a positive value and ends at another positive value; the mutual information starts from a positive value and ends at 0; the mutual information starts from 0, becomes positive for some time and ends at 0 (the bell form of the time dependence). In the context of the FMO complex study, the last case presents a special interest. Locally, we see phase transitions for some particular configurations. These cases are indicated by arrow in Fig.28 and Fig.29.
Figure 27. Holographic mutual information $I(A_0 \cup A_1; A_3)$, up to the normalizing factor, for the Vaidya metric in the four dimensional black brane background with $f = f(z, v)$ given by (2.20) and (2.22) ($m_0 = 0.25, m = 1$) and the $x_1$-projection of the 3 belts configuration shown in Fig.26, as function of the boundary time $t$ at fixed $l_1, l_2, l_3, x, y$. The lines of the same style correspond to the same $l_1, l_2, l_3$ and $y$, but different values of $x$, the distance between the sites "3" and "1" of the FMO complex. For more details see Fig.28 and Fig.29.

Figure 28. Detailed plots for Fig.27. In plots A: $l_1 = 0.3, l_2 = 0.8, l_3 = 0.7, y = 0.3$ and $0.2 < x < 0.24$; in plots B: $l_1 = 0.4, l_2 = 0.5, l_3 = 0.4, y = 0.3$ and $0.2 < x < 0.26$. Values of $x$ increase going from the top curve to the bottom one. Arrows indicate the phase transitions.
4.3 Matching holographic calculations to the simulation results.

In this subsection we fit some results of numerical simulations for the FMO complex presented in [50] by the holographic description. The mutual information at the physiological temperature ($300^\circ K$) calculated in [50], Fig.3c, when the first system is the site three and the second system is a mixed state of sites one and six is presented in Fig.29 by the red dashed line. The time dependence of the holographic mutual information $I(A_6 \cup A_1; A_3)$ increases going from the top curve to the bottom one. Arrow indicate the phase transitions.

Figure 29. Detailed plots for Fig.27. In plots A: $l_1 = 0.4, l_2 = 0.5, l_3 = 0.3, y = 0.3$ and $0.2 < x < 0.26$; B: $l_1 = 0.4, l_2 = 0.7, l_3 = 0.3, y = 0.3$ and $0.2 < x < 0.235$. Values of $x$ increase going from the top curve to the bottom one. C: $l_1 = 0.4, l_2 = 0.4, l_3 = 0.4, y = 0.3$ and $0.2 < x < 0.26$; D: $l_1 = 0.3, l_2 = 0.4, l_3 = 0.5, y = 0.3$ and $0.2 < x < 0.24$; E: $l_1 = 0.3, l_2 = 0.4, l_3 = 0.5, y = 0.3$ and $0.2 < x < 0.24$; F: $l_1 = 0.3, l_2 = 0.4, l_3 = 0.5, y = 0.3$ and $0.2 < x < 0.206$. Values of $x$ increase going from the top curve to the bottom one. Arrow indicate the phase transitions.
under the global quench by the Vaidya shell in AdS$_4$ is shown by the dark cyan line also in Fig.29. Note that we make rescaling for this line. We see a rather good fit of these two curves.

**Figure 30.** The dashed red curve shows the time dependence (in the logarithmic scale) of the mutual information at the physiological temperature (300°K) calculated in [50], Fig. 3c, when the fist system is the site ones and the second system is a mixed state of sites one and six. The time dependence of the holographic mutual information $I(A_6 \cup A_1; A_3)$ under the global quench by the Vaidya shell in AdS$_4$ is shown by the dark cyan line.

5 Conclusions

We have applied the holographic approach to evaluate the time dependence of entanglement entropy and quantum mutual information in the Fenna-Matthews-Olson protein-pigment complex in green sulfur bacteria during the transfer of an excitation from a chlorosome antenna to a reaction center. It is shown that the time evolution of the mutual information simulating the Lindblad master equation in some cases can be obtained by means of a dual gravity describing black hole formation in the Vaidya AdS spacetime or the Vaidya AdS black brane spacetime. The wake up and scrambling times for various partitions of the FMO complex are discussed. We have demonstrated that some results of numerical simulations [50] for the FMO complex can be fitted by reduced holographic models containing just 2 or 3 segments, Fig.21, Fig.23.B and Fig.30.

To describe another results known for the FMO complex it would be interesting to study more complex holographic models containing 7 or 8 segments. It would be also suitable in this context to change the geometry of disjoint regions and consider, for example, the disk regions. Considering the global AdS$_{d+1}$ one can also study the compact systems. In the case of the global AdS$_3$ one can consider the time dependence of the mutual information not only during the global quench, described by the Vaidya metric [66], but also during the local quench provided by ultrarelativistic particle in AdS$_3$ [67]. Studying Lifshitz backgrounds could be useful for describing not only the FMO complex but also other light-harvesting complexes. We suspect that the holographic approach could provide a useful description of certain appropriate quantities not only for quantum photosynthesis but also
for other life science phenomena studied in quantum biology such as the process of vision, the olfactory sense and quantum tunneling in biomolecules.

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