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Direct calculation of mutual information of distant regions

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ABSTRACT: We consider the (Rényi) mutual information, $I^{(n)}(A, B) = S_A^{(n)} + S_B^{(n)} - S_{A \cup B}^{(n)}$, of distant compact spatial regions A and B in the vacuum state of a free scalar field. The distance r between A and B is much greater than their sizes $R_{A,B}$. It is known that $I^{(n)}(A, B) \sim C_{AB}^{(n)} \langle 0 | \phi(r) \phi(0) | 0 \rangle^2$. We obtain the direct expression of $C_{AB}^{(n)}$ for arbitrary regions A and B. We perform the analytical continuation of n and obtain the mutual information. The direct expression is useful for the numerical computation. By using the direct expression, we can compute directly $I(A, B)$ without computing S_A, S_B and $S_{A \cup B}$ respectively, so it reduces significantly the amount of computation.

KEYWORDS: Field Theories in Higher Dimensions, Lattice Quantum Field Theory

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1 Introduction

The entanglement entropy in the quantum field theory plays important roles in many fields of physics including the string theory [1–13], condensed matter physics [14–17], lattice gauge theories [18, 19], cosmology [20], and the physics of the black hole [21–26]. The entanglement entropy is a useful quantity which characterizes quantum properties of given states.

For a given density matrix ρ of the total system, the entanglement entropy of the subsystem Ω is defined as

$$S_{\Omega} = -\text{Tr} \rho_{\Omega} \ln \rho_{\Omega}, \quad (1.1)$$

where $\rho_{\Omega} = \text{Tr}_{\Omega^c} \rho$ is the reduced density matrix of the subsystem Ω and Ω^c is the complement of Ω . The Rényi entropy $S_{\Omega}^{(n)}$ is defined as

$$S_{\Omega}^{(n)} = \frac{1}{1-n} \ln \text{Tr} \rho_{\Omega}^n. \quad (1.2)$$

The limit $n \rightarrow 1$ coincides with the entanglement entropy $\lim_{n \rightarrow 1} S_{\Omega}^{(n)} = S_{\Omega}$.

In this paper, we consider the (Rényi) mutual information, $I^{(n)}(A, B) = S_A^{(n)} + S_B^{(n)} - S_{A \cup B}^{(n)}$, of distant compact spatial regions A and B in the vacuum state of a free scalar

field. The distance r between A and B is much greater than their sizes $R_{A,B}$. It is known that [28], when $r \gg R_{A,B}$, the (Rényi) mutual information behaves as

$$I^{(n)}(A, B) \sim C_{AB}^{(n)} \langle 0 | \phi(r) \phi(0) | 0 \rangle^2, \quad (1.3)$$

where $C_{AB}^{(n)}$ depends on the shapes of the regions A and B . When both A and B are the spheres and the scalar field is massless, the coefficient $C_{AB}^{(n)}$ for a free scalar field was calculated analytically by Cardy [28]. However, it is difficult to calculate $C_{AB}^{(n)}$ analytically when both A and B are not the spheres or the scalar field is not massless. In this paper, we obtain the direct expression of $C_{AB}^{(n)}$ for arbitrary regions A and B in the vacuum state of a scalar field which has a general dispersion relation. We perform the analytical continuation of n and obtain the mutual information $I(A, B) = \lim_{n \rightarrow 1} I^{(n)}(A, B)$. The direct expression is useful for the numerical computation. By using the direct expression, we can compute directly $I(A, B)$ without computing S_A, S_B and $S_{A \cup B}$ respectively, so it reduces significantly the amount of computation.

We comment on the advantages of this direct expression over the conventional numerical computation by the real time formalism. Entanglement entropy in free scalar fields can be calculated numerically by the real time formalism [21, 22]. In order to calculate the coefficient $C_{AB}^{(n=1)}$ by the real time formalism, we have to plot the mutual information $I(A, B)$ as a function of r and extract the coefficient [26]. So we have to calculate numerically $S_{A \cup B}$ many times to plot $I(A, B)$ as a function of r . On the other hand, in our method, we separate the r dependence of $I(A, B)$ analytically and obtain the direct expression of $C_{AB}^{(n=1)}$. So, it reduces significantly the amount of computation.

To obtain the direct expression of $C_{AB}^{(n)}$, we use the operator method to compute the Rényi entropy developed in [29]. This operator method is based on the idea that $\text{Tr} \rho_\Omega^n$ is written as the expectation value of the local operator at Ω . This idea was originally used to compute $I^{(n)}(A, B)$ in the vacuum state by Cardy [28], Calabrese et al. [30] and Headrick [31]. This idea was generalized to an arbitrary density matrix ρ and the local operator was explicitly constructed in [29]. Cardy's work [28] was generalized (at least for the computation of the mutual information as opposed to the mutual Rényi information) for any CFT with a scalar in [38]. The next to leading terms in the long distance expansion of the mutual information in a free scalar theory was studied in [39]. The leading term for the mutual Rényi information for two widely separated identical compound systems in a free scalar theory was studied in [40].

The present paper is organized as follows. In section 2, we review the operator method to compute the Rényi entropy developed in [29]. In section 3, we expand the glueing operator which plays the important role in the operator method to compute the (Rényi) mutual information. In section 4, we compute the (Rényi) mutual information and obtain the direct expression of $C_{AB}^{(n)}$. In section 5, we apply our method to a massless free scalar field in $(d+1)$ dimension and perform numerical calculation for $d=2, 3$. We show that our method reproduces the results computed by the conventional real time formalism.

2 The review of the operator method to compute the Rényi entropy

We review the operator method to compute the Rényi entropy developed in [29]. We consider n copies of the scalar fields in $(d+1)$ dimensional spacetime and the j -th copy of the scalar field is denoted by $\{\phi^{(j)}\}$. Thus the total Hilbert space, $H^{(n)}$, is the tensor product of the n copies of the Hilbert space, $H^{(n)} = H \otimes H \cdots \otimes H$ where H is the Hilbert space of one scalar field. We define the density matrix $\rho^{(n)}$ in $H^{(n)}$ as

$$\rho^{(n)} \equiv \rho \otimes \rho \otimes \cdots \otimes \rho \quad (2.1)$$

where ρ is an arbitrary density matrix in H . We can express $\text{Tr} \rho_\Omega^n$ as

$$\text{Tr} \rho_\Omega^n = \text{Tr}(\rho^{(n)} E_\Omega), \quad (2.2)$$

where

$$\begin{aligned} E_\Omega = & \int \prod_{j=1}^n \prod_{x \in \Omega} D J^{(j)}(x) D K^{(j)}(x) \exp \left[i \int d^d x \sum_{l=1}^n J^{(l+1)}(x) \phi^{(l)}(x) \right] \\ & \times \exp \left[i \int d^d x \sum_{l=1}^n K^{(l)}(x) \pi^{(l)}(x) \right] \times \exp \left[-i \int d^d x \sum_{l=1}^n J^{(l)} \phi^{(l)} \right], \end{aligned} \quad (2.3)$$

where $\pi(x)$ is a conjugate momenta of $\phi(x)$, $[\phi(x), \pi(y)] = i\delta^d(x-y)$, and $J^{(j)}(x)$ and $K^{(j)}(x)$ exist only in Ω and $J^{(n+1)} = J^{(1)}$ and we normalize the measure of the functional integral as $\int D J^{(j)} \exp[i \int d^d x J^{(j)}(x) f(x)] = \prod_{x \in \Omega} \delta(f(x))$ where $f(x)$ is an arbitrary function. Notice that ϕ and π in (2.3) are operators and the ordering is important. This operator E_Ω is called as *the glueing operator*. When ρ is a pure state, $\rho = |\Psi\rangle \langle \Psi|$, the equation (2.2) becomes

$$\text{Tr} \rho_\Omega^n = \langle \Psi^{(n)} | E_\Omega | \Psi^{(n)} \rangle \quad (2.4)$$

where

$$|\Psi^{(n)}\rangle = |\Psi\rangle |\Psi\rangle \cdots |\Psi\rangle. \quad (2.5)$$

The useful property of the glueing operator for calculating the mutual information is the locality. When $\Omega = A \cup B$ and $A \cap B = \emptyset$,

$$E_{A \cup B} = E_A E_B. \quad (2.6)$$

From the locality (2.6), the mutual Rényi information in the vacuum state can be expressed as the correlation function of the glueing operators,

$$\frac{\text{Tr} \rho_{A \cup B}^{(n)}}{\text{Tr} \rho_A^{(n)} \text{Tr} \rho_B^{(n)}} = \frac{\langle 0^{(n)} | E_A E_B | 0^{(n)} \rangle}{\langle 0^{(n)} | E_A | 0^{(n)} \rangle \langle 0^{(n)} | E_B | 0^{(n)} \rangle}. \quad (2.7)$$

We consider $(d+1)$ dimensional free scalar field theory. For free scalar fields, it is useful to represent the glueing operator E_Ω in (2.3) as the normal ordered operator. We decompose ϕ and π into the creation and annihilation parts,

$$\phi(x) = \phi^+(x) + \phi^-(x), \quad \pi(x) = \pi^+(x) + \pi^-(x), \quad (2.8)$$

where

$$\begin{aligned}\phi^+(x) &= \int \frac{d^d p}{(2\pi)^d} \frac{1}{\sqrt{2E_p}} a_p e^{ipx}, & \phi^-(x) &= (\phi^+(x))^\dagger, \\ \pi^+(x) &= \int \frac{d^d p}{(2\pi)^d} (-i) \sqrt{\frac{E_p}{2}} a_p e^{ipx}, & \pi^-(x) &= (\pi^+(x))^\dagger,\end{aligned}\tag{2.9}$$

here E_p is the energy and $[a_p, a_{p'}^\dagger] = (2\pi)^d \delta^d(p-p')$. The commutators of these operators are

$$\begin{aligned}[\phi^+(x), \phi^-(y)] &= \langle 0 | \phi(x) \phi(y) | 0 \rangle = \int \frac{d^d p}{(2\pi)^d} \frac{1}{2E_p} e^{ip(x-y)} \equiv \frac{1}{2} W^{-1}(x, y), \\ [\pi^+(x), \pi^-(y)] &= \langle 0 | \pi(x) \pi(y) | 0 \rangle = \int \frac{d^d p}{(2\pi)^d} \frac{E_p}{2} e^{ip(x-y)} \equiv \frac{1}{2} W(x, y), \\ [\pi^+(x), \phi^-(y)] &= [\pi^-(x), \phi^+(y)] = -\frac{i}{2} \delta^d(x-y),\end{aligned}\tag{2.10}$$

where we have defined the matrices W and W^{-1} which has continuous indices x, y in (2.10) and W^{-1} is the inverse of W . W and W^{-1} are positive definite symmetric matrices. By using (2.10) and the Baker-Campbell-Hausdorff (BCH) formula $e^X e^Y = e^{[X,Y]} e^Y e^X$, $e^{X+Y} = e^{-\frac{1}{2}[X,Y]} e^X e^Y$, for $[[X, Y], X] = [[X, Y], Y] = 0$, we obtain

$$\begin{aligned}& \exp \left[i \int d^d x J' \phi \right] \exp \left[i \int d^d x K \pi \right] \exp \left[-i \int d^d x J \phi \right] \\ &= : \exp \left[i \int d^d x (K \pi + (J' - J) \phi) \right] : \\ & \times \exp \left[\int d^d x d^d y \left(-\frac{1}{4} K(x) A(x, y) K(y) - \frac{1}{4} (J' - J)(x) D(x, y) (J' - J)(y) \right) \right. \\ & \quad \left. - \int d^d x \frac{i}{2} K(x) (J' + J)(x) \right],\end{aligned}\tag{2.11}$$

where $: O :$ means the normal ordered operator of O . From (2.11) we can rewrite E_Ω in (2.3) as the normal ordered operator,

$$E_\Omega = \int \prod_{j=1}^n \prod_{x \in \Omega} D J^{(j)}(x) D K^{(j)}(x) : \exp \left[i \sum_{l=1}^n \int d^d x ((J^{(l+1)} - J^{(l)}) \phi^{(l)} + K^{(l)} \pi^{(l)}) \right] : \exp[-\tilde{S}],\tag{2.12}$$

where $J^{(n+1)} = J^{(1)}$ and

$$\begin{aligned}\tilde{S} &\equiv \sum_{l=1}^n \left[\int d^d x d^d y \left[\frac{1}{4} K^{(l)}(x) W(x, y) K^{(l)}(y) + \frac{1}{4} (J^{(l+1)} - J^{(l)})(x) W^{-1}(x, y) (J^{(l+1)} - J^{(l)})(y) \right] \right. \\ & \quad \left. + \frac{i}{2} \int d^d x K^{(l)}(x) (J^{(l+1)} + J^{(l)})(x) \right].\end{aligned}\tag{2.13}$$

3 The expansion of the glueing operator

We consider a complex scalar field ϕ because it is useful for later calculation. The mutual information of a real free scalar field can be obtained by dividing the mutual information

of the complex free scalar field by 2. Then, the glueing operator becomes

$$E_\Omega = \int \prod_{j=0}^{n-1} \prod_{x \in \Omega} DJ^{(j)}(x) DK^{(j)}(x) : \exp \left[i \sum_{l=0}^{n-1} \int d^d x ((J^{(l+1)} - J^{(l)})\phi^{(l)*} + K^{(l)}\pi^{(l)*} + (J^{(l+1)*} - J^{(l)*})\phi^{(l)} + K^{(l)*}\pi^{(l)}) \right] : \exp[-\tilde{S}], \quad (3.1)$$

where

$$\begin{aligned} \tilde{S} \equiv & \sum_{l=0}^{n-1} \left[\int d^d x d^d y \left[\frac{1}{2} K^{(l)}(x) A(x, y) K^{(l)*}(y) + \frac{1}{2} (J^{(l+1)} - J^{(l)})(x) D(x, y) (J^{(l+1)*} - J^{(l)*})(y) \right] \right. \\ & \left. + \frac{i}{2} \int d^d x (K^{(l)}(x) (J^{(l+1)*} + J^{(l)*})(x) + K^{(l)*}(x) (J^{(l+1)} + J^{(l)})(x)) \right]. \end{aligned} \quad (3.2)$$

For the free scalar field, it is useful to use the following Fourier transformation,

$$f^{(l)} = \frac{1}{\sqrt{n}} \sum_{k=0}^{n-1} e^{2\pi i k l / n} \tilde{f}^{(k)} \quad (3.3)$$

where $f^{(l)}$ is an arbitrary n dimensional vector and $\tilde{f}^{(k)}$ is its Fourier transformation, i.e. (3.3) is the definition of the Fourier transformation. The Fourier transformation diagonalizes the glueing operator,

$$E_\Omega = \prod_{k=0}^{n-1} E_\Omega^{(k)} \quad (3.4)$$

where

$$E_\Omega^{(k)} = \int \prod_{x \in \Omega} D\tilde{J}^{(k)}(x) D\tilde{K}^{(k)}(x) : \exp[iQ^{(k)}] : \exp[-\tilde{S}^{(k)}] \quad (3.5)$$

$$Q^{(k)} \equiv \int d^d x [(e^{2\pi i k / n} - 1) \tilde{J}^{(k)} \tilde{\phi}^{(k)*} + (e^{-2\pi i k / n} - 1) \tilde{J}^{(k)*} \tilde{\phi}^{(k)} + \tilde{K}^{(k)} \tilde{\pi}^{(k)*} + \tilde{K}^{(k)*} \tilde{\pi}^{(k)}] \quad (3.6)$$

$$\begin{aligned} \tilde{S}^{(k)} \equiv & \int d^d x d^d y \left[\frac{1}{2} \tilde{K}^{(k)}(x) A(x, y) \tilde{K}^{(k)*}(y) + \frac{1}{2} \left(1 - \cos\left(\frac{2\pi k}{n}\right) \right) \tilde{J}^{(k)}(x) D(x, y) \tilde{J}^{(k)*}(y) \right] \\ & + \frac{i}{2} \int d^d x ((e^{-2\pi i k / n} + 1) \tilde{K}^{(k)}(x) \tilde{J}^{(k)*}(x) + (e^{2\pi i k / n} + 1) \tilde{K}^{(k)*}(x) \tilde{J}^{(k)}(x)). \end{aligned} \quad (3.7)$$

In order to expand $: \exp[iQ^{(k)}] :$ in $E_\Omega^{(k)}$, we define $\langle \dots \rangle$ as

$$\langle \dots \rangle \equiv \frac{\int \prod_{x \in \Omega} D\tilde{J}^{(k)}(x) D\tilde{K}^{(k)}(x) \exp[-\tilde{S}^{(k)}] \dots}{\int \prod_{x \in \Omega} D\tilde{J}^{(k)}(x) D\tilde{K}^{(k)}(x) \exp[-\tilde{S}^{(k)}]} \quad (3.8)$$

where $\dots$ is an arbitrary function of $\tilde{J}^{(k)}$ and $\tilde{K}^{(k)}$. When Ω is a compact spatial region, we express $E_\Omega^{(k)}$ as a sum of the local operators at a conventionally chosen point x_0 inside

Ω . Thus, we expand $E_\Omega^{(k)}$ as

$$\begin{aligned} \frac{E_\Omega^{(k)}}{\langle 0|E_\Omega^{(k)}|0\rangle} &= 1 - \frac{1}{2} \langle : (Q^{(k)})^2 : \rangle + \dots \\ &= 1 - \left(2 - 2 \cos \left(\frac{2\pi k}{n} \right) \right) \int d^d x d^d y \langle \tilde{J}^{(k)}(x) \tilde{J}^{(k)*}(y) \rangle : \tilde{\phi}^{(k)*}(x) \tilde{\phi}^{(k)}(y) : + \dots \\ &= 1 - : \tilde{\phi}^{(k)*}(x_0) \tilde{\phi}^{(k)}(x_0) : \left(2 - 2 \cos \left(\frac{2\pi k}{n} \right) \right) \int d^d x d^d y \langle \tilde{J}^{(k)}(x) \tilde{J}^{(k)*}(y) \rangle + \dots \end{aligned} \quad (3.9)$$

In the last line in (3.9), we expanded the operator $: \tilde{\phi}^{(k)*}(x) \tilde{\phi}^{(k)}(y) :$ around x_0 and took it outside the integral because we consider the case that Ω is a compact spatial region and this expansion is useful for the later computation of the Rényi mutual information. In order to represent the Gauss integrals of $\tilde{K}^{(k)}$ and $\tilde{J}^{(k)}$, we will use the following matrix notation,

$$W(x, y) = \begin{pmatrix} W(x_\Omega, y_\Omega) & W(x_\Omega, y_{\Omega^c}) \\ W(x_{\Omega^c}, y_\Omega) & W(x_{\Omega^c}, y_{\Omega^c}) \end{pmatrix} \equiv \begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \quad (3.10)$$

$$W^{-1}(x, y) = \begin{pmatrix} W^{-1}(x_\Omega, y_\Omega) & W^{-1}(x_\Omega, y_{\Omega^c}) \\ W^{-1}(x_{\Omega^c}, y_\Omega) & W^{-1}(x_{\Omega^c}, y_{\Omega^c}) \end{pmatrix} \equiv \begin{pmatrix} D & E \\ E^T & F \end{pmatrix} \quad (3.11)$$

where $x_{\Omega(\Omega^c)}$ and $y_{\Omega(\Omega^c)}$ are the coordinates in $\Omega(\Omega^c)$, where Ω^c is the complement of Ω .

In order to calculate $\langle \tilde{J}^{(k)}(x) \tilde{J}^{(k)*}(y) \rangle$, we perform the $\tilde{K}^{(k)}$ integral first,

$$\begin{aligned} &\int \prod_{x \in \Omega} D \tilde{K}^{(k)}(x) \exp[-\tilde{S}^{(k)}] \\ &= \frac{1}{\det \left(\frac{A}{2\pi} \right)} \exp \left[- \int d^d x d^d y \tilde{J}^{(k)*}(x) \left(A^{-1} + D + \cos \left(\frac{2\pi k}{n} \right) (A^{-1} - D) \right) (x, y) \tilde{J}^{(k)}(y) \right]. \end{aligned} \quad (3.12)$$

From (3.12), we obtain

$$\begin{aligned} \langle \tilde{J}^{(k)}(x) \tilde{J}^{(k)*}(y) \rangle &= \frac{\int \prod_{x \in \Omega} D \tilde{J}^{(k)}(x) D \tilde{K}^{(k)}(x) \exp[-\tilde{S}^{(k)}] \tilde{J}^{(k)}(x) \tilde{J}^{(k)*}(y)}{\int \prod_{x \in \Omega} D \tilde{J}^{(k)}(x) D \tilde{K}^{(k)}(x) \exp[-\tilde{S}^{(k)}]} \\ &= \left(A^{-1} + D + \cos \left(\frac{2\pi k}{n} \right) (A^{-1} - D) \right)^{-1} (x, y). \end{aligned} \quad (3.13)$$

In order to separate the n dependence of $\langle \tilde{J}^{(k)}(x) \tilde{J}^{(k)*}(y) \rangle$, we rewrite it as

$$\left(A^{-1} + D + \cos \left(\frac{2\pi k}{n} \right) (A^{-1} - D) \right)^{-1} = X \left(1 - \cos \left(\frac{2\pi k}{n} \right) Y \right)^{-1} X \quad (3.14)$$

where

$$X \equiv (A^{-1} + D)^{-1/2}, \quad Y \equiv X(D - A^{-1})X \quad (3.15)$$

$$Y = O^T \Lambda O, \quad \Lambda = \text{diag}(\lambda_i) \quad (3.16)$$

Thus we obtain

$$\left(X \left(1 - \cos \left(\frac{2\pi k}{n} \right) Y \right)^{-1} X \right)_{i,j} = \sum_l Z_{li} \frac{1}{1 - \lambda_l \cos \left(\frac{2\pi k}{n} \right)} Z_{lj} \quad (3.17)$$

where $Z = OX$ and we discretized the space coordinates in order to regularize the scalar field. In the appendix A, we show that the range of the eigenvalues λ_i is

$$0 \leq \lambda_i < 1. \quad (3.18)$$

Finally, when Ω is a compact spatial region, we obtain the expansion of $E_\Omega^{(k)}$ as

$$\frac{E_\Omega^{(k)}}{\langle 0 | E_\Omega^{(k)} | 0 \rangle} = 1 - : \tilde{\phi}^{(k)*}(x_0) \tilde{\phi}^{(k)}(x_0) : C_\Omega^{(k)} + \cdots, \quad (3.19)$$

where

$$\begin{aligned} C_\Omega^{(k)} &\equiv \left(2 - 2 \cos \left(\frac{2\pi k}{n} \right) \right) \int d^d x d^d y \langle \tilde{J}^{(k)}(x) \tilde{J}^{(k)*}(y) \rangle \\ &= \left(2 - 2 \cos \left(\frac{2\pi k}{n} \right) \right) \sum_i \sum_j \sum_l Z_{li} \frac{1}{1 - \lambda_l \cos \left(\frac{2\pi k}{n} \right)} Z_{lj} \\ &\equiv \left(2 - 2 \cos \left(\frac{2\pi k}{n} \right) \right) \sum_{i_\Omega} \sum_{j_\Omega} \sum_{l_\Omega} Z_{l_\Omega i_\Omega}^{(\Omega)} \frac{1}{1 - \lambda_{l_\Omega}^{(\Omega)} \cos \left(\frac{2\pi k}{n} \right)} Z_{l_\Omega j_\Omega}^{(\Omega)}. \end{aligned} \quad (3.20)$$

In the last line in (3.20), we added the subscript and the superscript Ω in order to clarify that i_Ω , j_Ω and l_Ω are the coordinates in Ω , and $Z^{(\Omega)}$ and $\lambda^{(\Omega)}$ depend on Ω .

4 The (Rényi) mutual information of distant regions

We apply above results to the mutual Rényi information $I^{(n)}(A, B)$ of disjoint compact spatial regions A and B in the vacuum states of the free scalar field. From (2.7), (3.4) and (3.19), we obtain

$$\begin{aligned} \frac{\text{Tr} \rho_{A \cup B}^n}{\text{Tr} \rho_A^n \text{Tr} \rho_B^n} &= \prod_{k=0}^{n-1} \frac{\langle 0 | E_A^{(k)} E_B^{(k)} | 0 \rangle}{\langle 0 | E_A^{(k)} | 0 \rangle \langle 0 | E_B^{(k)} | 0 \rangle} \\ &\simeq \prod_{k=0}^{n-1} \langle 0 | (1 - : \tilde{\phi}^{(k)*}(x_A) \tilde{\phi}^{(k)}(x_A) : C_A^{(k)}) (1 - : \tilde{\phi}^{(k)*}(x_B) \tilde{\phi}^{(k)}(x_B) : C_B^{(k)}) | 0 \rangle \\ &= \prod_{k=0}^{n-1} (1 + C_A^{(k)} C_B^{(k)} f(r)) \end{aligned} \quad (4.1)$$

where x_A and x_B are some conventionally chosen points inside A and B , $r = |x_A - x_B|$, and

$$\begin{aligned} f(r) &\equiv \langle 0 | : \tilde{\phi}^{(k)*}(x_A) \tilde{\phi}^{(k)}(x_A) :: \tilde{\phi}^{(k)*}(x_B) \tilde{\phi}^{(k)}(x_B) : | 0 \rangle \\ &= (\langle 0 | \phi(x_A) \phi^*(x_B) | 0 \rangle)^2 \end{aligned} \quad (4.2)$$

From (4.1), we obtain the mutual Rényi information as

$$I^{(n)}(A, B) = \frac{1}{n-1} \ln \frac{\text{Tr} \rho_{A \cup B}^n}{\text{Tr} \rho_A^n \text{Tr} \rho_B^n} \simeq \frac{1}{n-1} \sum_{k=0}^{n-1} \ln \left(1 + C_A^{(k)} C_B^{(k)} f(r) \right) \simeq \frac{f(r)}{n-1} \sum_{k=0}^{n-1} C_A^{(k)} C_B^{(k)} \quad (4.3)$$

We substitute $C_{\Omega}^{(k)}$ in (3.20) into (4.3) and obtain

$$I^{(n)}(A, B) \simeq C_{AB}^{(n)} f(r), \quad (4.4)$$

$$C_{AB}^{(n)} \equiv \frac{4}{n-1} \sum_{i_A} \sum_{j_A} \sum_{l_A} \sum_{i_B} \sum_{j_B} \sum_{l_B} Z_{l_A i_A}^{(A)} Z_{l_A j_A}^{(A)} Z_{l_B i_B}^{(B)} Z_{l_B j_B}^{(B)} F(n, \lambda_{l_A}^{(A)}, \lambda_{l_B}^{(B)}), \quad (4.5)$$

where

$$F(n, a, b) \equiv \sum_{k=0}^{n-1} \left(1 - \cos \left(\frac{2\pi k}{n} \right) \right)^2 \frac{1}{1 - a \cos \left(\frac{2\pi k}{n} \right)} \frac{1}{1 - b \cos \left(\frac{2\pi k}{n} \right)}. \quad (4.6)$$

We can perform explicitly the summation in (4.6) and obtain (see appendix B)

$$\begin{aligned} F(n, a, b) = n \frac{(1+p^2)(1+q^2)}{4pq} & \left[2 - \frac{(1-p)(1+p^n)}{(1+p)(1-p^n)} - \frac{(1-q)(1+q^n)}{(1+q)(1-q^n)} \right. \\ & + \frac{2}{(1+p)(1+q)(p-q)(1-pq)} \left\{ \frac{1-p}{1-p^n} p(1-q)^2(1+q) - \frac{1-q}{1-q^n} q(1-p)^2(1+p) \right. \\ & \left. \left. - (p-q)(1+pq - (p+q)pq) \right\} \right] \end{aligned} \quad (4.7)$$

where

$$p \equiv \rho(a) = \frac{1}{a} \left(1 - \sqrt{1-a^2} \right), \quad q \equiv \rho(b) = \frac{1}{b} \left(1 - \sqrt{1-b^2} \right). \quad (4.8)$$

From (4.7), for $n = 1, 2, 3$ and 4 , we obtain

$$F(n=1, a, b) = 0 \quad (4.9)$$

$$F(n=2, a, b) = 4 \frac{(1+p^2)}{(1+p)^2} \frac{(1+q^2)}{(1+q)^2} \quad (4.10)$$

$$F(n=3, a, b) = \frac{9}{2} \frac{1+p^2}{1+p+p^2} \frac{1+q^2}{1+q+q^2} \quad (4.11)$$

$$F(n=4, a, b) = 2 \left[1 + 2 \frac{(1+p^2)}{(1+p)^2} \frac{(1+q^2)}{(1+q)^2} \right]. \quad (4.12)$$

When $n = 2, 3$, $F(n, a, b)$ is a product of the function of a and b and $C_{AB}^{(n)}$ becomes,

$$C_{AB}^{(n)} = \tilde{C}_A^{(n)} \tilde{C}_B^{(n)}, \quad (n = 2, 3) \quad (4.13)$$

where $\tilde{C}_{A(B)}^{(n)}$ is a function which is determined by the shape of $A(B)$. So, when $n = 2, 3$, $C_{AB}^{(n)}$ is not entangled, i.e. it is a simple product of functions each of which is determined by the shape of $A(B)$. In general, $F(n, a, b)$ is not a product of the function of a and b and $C_{AB}^{(n)}$ is entangled. However, we will compute $C_{AB}^{(n)}$ numerically later and show that $C_{AB}^{(n)}$ is factorized in a $(d+1)$ dimensional massless free scalar field for $d = 2, 3$. This factorization is not clear in the formal expressions in (4.7) and numerical calculation is important to check the factorization.

Because $F(n, a, b)$ is an elementary function of n , its analytical continuation is trivial. So we can take $n \rightarrow 1$ limit in $C_{AB}^{(n)}$ in (4.5). From (4.7) and (4.9), we obtain

$$C_{AB}^{(n=1)} = 4 \sum_{i_A} \sum_{j_A} \sum_{l_A} \sum_{i_B} \sum_{j_B} \sum_{l_B} Z_{l_A i_A}^{(A)} Z_{l_A j_A}^{(A)} Z_{l_B i_B}^{(B)} Z_{l_B j_B}^{(B)} \left(\frac{\partial}{\partial n} F(n, \lambda_{l_A}^{(A)}, \lambda_{l_B}^{(B)}) \right) \Big|_{n=1}, \quad (4.14)$$

where

$$\left(\frac{\partial}{\partial n} F(n, a, b) \right) \Big|_{n=1} = \frac{1}{2} \frac{(1+p^2)(1+q^2)}{(1+p)(1+q)(p-q)(1-pq)} [(1-p)(1+q) \ln p - (1+p)(1-q) \ln q]. \quad (4.15)$$

The calculation of the matrix Z and the eigenvalues λ_i is simple matrix computation. So, we can compute $C_{AB}^{(n=1)}$ numerically. Note that (4.4) is the mutual information of a free complex scalar field and the mutual information of a free real scalar field is a half of (4.4).

5 Massless free scalar field theory in $(d+1)$ dimension

5.1 Lattice formulation

We apply the above formalism to a massless free scalar field in $(d+1)$ -dimensional Minkowski spacetime. The Lagrangian is given by

$$L = \int d^d x \frac{1}{2} [\dot{\phi}^2 - (\nabla \phi)^2]. \quad (5.1)$$

As an ultraviolet regulator, we replace the continuous d -dimensional space coordinates x by a lattice of discrete points with spacing a . As an infrared cutoff, we allow the individual components of $n \equiv x/a$ to assume only a finite number N of independent values $-N/2 < n_\mu \leq N/2$. The Greek indices denoting vector quantities run from one to d . Outside this range we assume the lattice is periodic. The dimensionless Hamiltonian $H_0 \equiv aH$ is given by

$$H_0 \equiv aH = \sum_n \left[\frac{1}{2} \pi_n^2 + \frac{1}{2} \sum_{\mu=1}^d (\phi_{n_\nu + \delta_{\nu\mu}} - \phi_{n_\nu})^2 + \frac{a^2 m^2}{2} \phi_n^2 \right] \equiv \sum_n \frac{1}{2} \pi_n^2 + \sum_{m,n} \frac{1}{2} \phi_m V_{mn} \phi_n, \quad (5.2)$$

where ϕ_n and π_n are dimensionless and Hermitian, and obey the canonical commutation relations

$$[\phi_n, \pi_m] = i\delta_{nm}. \quad (5.3)$$

In eq. (5.2) we insert a mass term in order to remove a zero eigenvalue of V_{mn} ; if V_{mn} should have the zero eigenvalue, W^{-1} in (2.10) would not exist. Later we will take N to infinity. In this limit we can neglect the zero eigenvalue of V_{mn} and will take am to zero.

From (5.2) we obtain (see e.g. [27])

$$W_{mn} = N^{-d} \sum_k \left[a^2 m^2 + 2 \sum_{\mu=1}^d \left(1 - \cos \frac{2\pi k_\mu}{N} \right) \right]^{1/2} e^{2\pi i k(n-m)/N}, \quad (5.4)$$

$$W_{mn}^{-1} = N^{-d} \sum_k \left[a^2 m^2 + 2 \sum_{\mu=1}^d \left(1 - \cos \frac{2\pi k_\mu}{N} \right) \right]^{-1/2} e^{2\pi i k(n-m)/N}, \quad (5.5)$$

where the index k also carries d integer valued components, each in the range of $-N/2 < k_\mu \leq N/2$. We take N to infinity and change the momentum sum into an integral with the

replacements $q_\mu = 2\pi k_\mu/N$ and $N^{-d} \sum_k \rightarrow \int_{-\pi}^{\pi} \frac{d^d q}{(2\pi)^d}$, and then we have

$$W_{mn} = \int_{-\pi}^{\pi} \frac{d^d q}{(2\pi)^d} e^{iq(n-m)} \left[a^2 m^2 + 2 \sum_{\mu=1}^d (1 - \cos q_\mu) \right]^{\frac{1}{2}}, \quad (5.6)$$

$$W_{mn}^{-1} = \int_{-\pi}^{\pi} \frac{d^d q}{(2\pi)^d} e^{iq(n-m)} \left[a^2 m^2 + 2 \sum_{\mu=1}^d (1 - \cos q_\mu) \right]^{\frac{-1}{2}}. \quad (5.7)$$

In (5.6) and (5.7) the integrals converge when $am \rightarrow 0$, so we can take am to zero,

$$W_{mn} = \int_{-\pi}^{\pi} \frac{d^d q}{(2\pi)^d} e^{iq(n-m)} \left[2 \sum_{\mu=1}^d (1 - \cos q_\mu) \right]^{\frac{1}{2}}, \quad (5.8)$$

$$W_{mn}^{-1} = \int_{-\pi}^{\pi} \frac{d^d q}{(2\pi)^d} e^{iq(n-m)} \left[2 \sum_{\mu=1}^d (1 - \cos q_\mu) \right]^{\frac{-1}{2}}. \quad (5.9)$$

From (5.8) and (5.9) we can compute W_{mn} and W_{mn}^{-1} numerically. From (2.10) and (4.2), we obtain $f(r) = \frac{1}{4}(W^{-1}(x, y))^2$. So we need to calculate W_{mn}^{-1} for $\|n - m\| \gg 1$. The integrands in (5.8) and (5.9) highly oscillate when $\|n - m\| \gg 1$, and the numerical integrals converge very slowly. We can obtain approximate expressions of W_{mn} and W_{mn}^{-1} by hand when $\|n - m\| \gg 1$ [26]. To evaluate W_{mn} and W_{mn}^{-1} when $\|n - m\| \gg 1$, we define $r \equiv a(n - m)$ and take $\|n - m\|$ to infinity keeping r fixed. We change the variable as $p = q/a$, and then we have

$$W_{mn} = a^d \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d p}{(2\pi)^d} e^{ipr} \left[2 \sum_{\mu=1}^d (1 - \cos ap_\mu) \right]^{\frac{1}{2}} \rightarrow a^{d+1} \int_{-\infty}^{\infty} \frac{d^d p}{(2\pi)^d} e^{ipr - \frac{a}{\pi} \|p\|} [\|p\|^2]^{\frac{1}{2}}. \quad (5.10)$$

We can perform the integral in (5.10) analytically when $\|r\|/a \rightarrow \infty$ (see appendix A of [25]), and then we obtain

$$W_{mn} \rightarrow a^{d+1} \frac{A_d}{\|r\|^{d+1}} = \frac{A_d}{\|n - m\|^{d+1}}, \quad (5.11)$$

where

$$A_d = \begin{cases} -\frac{(d-1)!!}{(2\pi)^{d/2}} & \text{for even } d \geq 2, \\ -\frac{(d-1)!!}{(2\pi)^{(d+1)/2}} & \text{for odd } d \geq 3. \end{cases} \quad (5.12)$$

We can evaluate W_{mn}^{-1} when $\|n - m\| \gg 1$ in the same way (see appendix A of [25]), and then we obtain

$$W_{mn}^{-1} \rightarrow a^{d-1} \int_{-\infty}^{\infty} \frac{d^d p}{(2\pi)^d} e^{ipr - \frac{a}{\pi} \|p\|} [\|p\|^2]^{\frac{-1}{2}} \rightarrow a^{d-1} \frac{B_d}{\|r\|^{d-1}} = \frac{B_d}{\|n - m\|^{d-1}}. \quad (5.13)$$

Figure 1. The coefficient $C_{AB}^{(n)}$ as a function of R^4 , where $C_{AB}^{(n)}$ is the coefficient of the (Rényi) mutual information $I^{(n)}(A, B)$ of two spheres A and B whose radii are $R_A = R_B \equiv R$. The lines are the best linear fit.

where

$$B_d = \begin{cases} \frac{(d-3)!!}{(2\pi)^{d/2}} & \text{for even } d \geq 2, \\ 2 \frac{(d-3)!!}{(2\pi)^{(d+1)/2}} & \text{for odd } d \geq 3, \end{cases} \quad (5.14)$$

where $0!! = (-1)!! = 1$.

From (2.10), (4.2), (4.4) and (5.13), we obtain

$$I^{(n)}(A, B) \simeq C_{AB}^{(n)} \frac{B_d^2}{4 \|n - m\|^{2d-2}}, \quad (5.15)$$

where $C_{AB}^{(n)}$ is defined in (4.5). Note that the lattice spacing a is canceled out because the (Rényi) mutual information is dimensionless. So we calculate $C_{AB}^{(n)}$ in (5.15) by using the dimensionless matrices W_{mn} and W_{mn}^{-1} .

5.2 Numerical calculations

We calculate numerically the (Rényi) mutual information $I^{(n)}(A, B)$ of two spheres A and B whose radii are $R_A = R_B \equiv R$, and the distance between the centers of them is r for $d = 3$. We put the centers of the spheres on a lattice. We define the sphere as a set of points which are at distances of $\tilde{R}$ or less from the center of the sphere. In order to reduce the effect of the discretization, we correct $\tilde{R}$ and define the radius of this sphere as $R := (3V/4\pi)^{1/3}$ where V is a number of points in the sphere.

We show the computed values of $C_{AB}^{(n)}$ in (5.15) as a function of R^4 in figure 1. As can be seen, $C_{AB}^{(n)}$ is proportional to R^4 .

Thus, we obtain

$$I^{(n)}(A, B) \simeq g_{AB}^{(n)} \frac{R^4}{r^4}, \quad (5.16)$$

where $g_{AB}^{(n)}$ is a dimensionless constant. We calculate the coefficient $g_{AB}^{(n)}$ from slopes of graphs of $C_{AB}^{(n)}$ as a function of R^4 . We show the computed values of $g_{AB}^{(n)}$ as a function of n in figure 2.

Figure 2. The coefficient $g_{AB}^{(n)}$ in (5.16) as a function of n . We show the values of $g_{AB}^{(n)}$ computed by the direct calculation developed in this paper and the real time formalism, and the theoretical values $g_{AB}^{(n)}|_{d=3} = \frac{n^4-1}{15n^3(n-1)}$.

For comparison, we also showed the values of $g_{AB}^{(n)}$ computed by the real time formalism [21] and the theoretical values $g_{AB}^{(n)}|_{d=3} = \frac{n^4-1}{15n^3(n-1)}$ obtained by Cardy [28]. In order to calculate the coefficient $g_{AB}^{(n)}$ by the real time formalism, we plotted the (Rényi) mutual information $I^{(n)}(A, B)$ as a function of r and extract the coefficient in the same way as the mutual information [26]. From figure 2, for $n = 1$, the value of $g_{AB}^{(n)}$ computed by the direct calculation and one computed by the real time formalism and theoretical one are almost equal. For $n > 1$, the values of $g_{AB}^{(n)}$ computed by the direct calculation and those computed by the real time formalism are almost equal, however, the theoretical values $g_{AB}^{(n)}|_{d=3}$ are slightly larger than numerical computed values. The discrepancy for $n > 1$ probably indicates that the effect of the discretization become important when n increases. The direct calculation of the (Rényi) mutual information developed in this paper reproduces the results obtained by the conventional real time formalism. The direct calculation reduces significantly the amount of computation.

Next, we consider whether the coefficient $C_{AB}^{(n)}$ is factorized or not. We computed $h^{(n)}(A, B) \equiv \frac{(C_{AB}^{(n)})^2}{C_{AA}^{(n)}C_{BB}^{(n)}}$ in some cases. If $C_{AB}^{(n)}$ is factorized, $h^{(n)}(A, B) = 1$. For $n = 1, 2, \dots, 20$, we obtained the result that $h^{(n)}(A, B)$ is almost equal to 1 when A is a sphere and B is a cube and when A is a cube and B is a cube in the center of which there is a cubic hollow and when A is a cube in the center of which there is a cubic hollow and the shape of B is the same as the shape of A and the size of B is different from the size of A . These results suggest that the coefficient $C_{AB}^{(n)}$ is factorized in a massless free scalar field in $(3+1)$ dimension. This factorization is not clear in the formal expressions in (4.7) and (4.15) and numerical calculation is important to check the factorization.

For $d = 2$, we calculate numerically the (Rényi) mutual information $I^{(n)}(A, B)$ of two disks A and B whose radii are $R_A = R_B \equiv R$, and the distance between the centers of them is r for $d = 2$. We put the centers of the disks on a lattice. We define the disk as a set of points which are at distances of $\tilde{R}$ or less from the center of the disk. In order to reduce the effect of the discretization, we correct $\tilde{R}$ and define the radius of this disk as $R := (S/\pi)^{1/2}$ where S is a number of points in the disk.

Figure 3. The coefficient $C_{AB}^{(n)}$ as a function of R^2 , where $C_{AB}^{(n)}$ is the coefficient of the (Rényi) mutual information $I^{(n)}(A, B)$ of two disks A and B whose radii are $R_A = R_B \equiv R$. The lines are the best linear fit.

Figure 4. The coefficient $g_{AB}^{(n)}$ in (5.17) as a function of n . We show the values of $g_{AB}^{(n)}$ computed by the direct calculation developed in this paper and the real time formalism, and the theoretical values $g_{AB}^{(n)}|_{d=2}$ in (5.18).

We show the computed values of $C_{AB}^{(n)}$ in (5.15) as a function of R^2 in figure 3. As can be seen, $C_{AB}^{(n)}$ is proportional to R^2 .

Thus, we obtain

$$I^{(n)}(A, B) \simeq g_{AB}^{(n)} \frac{R^2}{r^2}, \quad (5.17)$$

where $g_{AB}^{(n)}$ is a dimensionless constant. We calculate the coefficient $g_{AB}^{(n)}$ from slopes of graphs of $C_{AB}^{(n)}$ as a function of R^2 . We show the computed values of $g_{AB}^{(n)}$ as a function of n in figure 4.

For comparison, we also showed the values of $g_{AB}^{(n)}$ computed by the real time formalism [21] and the theoretical values,

$$g_{AB}^{(n)}|_{d=2} = \frac{n}{2\pi^2(n-1)} \int_0^\infty \int_0^\infty \left(\frac{(1-x)(1-y)(1-(xy)^{n-1})}{1-xy} + (1-x^{n-1})(1-y^{n-1}) \right) dx dy \times \frac{1}{(1+x)(1+y)(1-x^n)(1-y^n)}, \quad (5.18)$$

obtained by Cardy [28]. In order to calculate the coefficient $g_{AB}^{(n)}$ by the real time formalism, we plotted the (Rényi) mutual information $I^{(n)}(A, B)$ as a function of r and extract the coefficient in the same way as the mutual information [26]. From figure 4, for $n = 1$,

the value of $g_{AB}^{(n)}$ computed by the direct calculation and one computed by the real time formalism and theoretical one are almost equal. For $n > 1$, the values of $g_{AB}^{(n)}$ computed by the direct calculation and those computed by the real time formalism are almost equal, however, the theoretical values $g_{AB}^{(n)}|_{d=2}$ are slightly larger than numerical computed values. The discrepancy for $n > 1$ probably indicates that the effect of the discretization become important when n increases. The direct calculation of the (Rényi) mutual information developed in this paper reproduces the results obtained by the conventional real time formalism. The direct calculation reduces significantly the amount of computation.

Next, we consider whether the coefficient $C_{AB}^{(n)}$ is factorized or not. We computed $h^{(n)}(A, B) \equiv \frac{(C_{AB}^{(n)})^2}{C_{AA}^{(n)}C_{BB}^{(n)}}$ in some cases. If $C_{AB}^{(n)}$ is factorized, $h^{(n)}(A, B) = 1$. For $n = 1, 2, \dots, 20$, we obtained the result that $h^{(n)}(A, B)$ is almost equal to 1 when A is a disk and B is a square and when A is a square and B is a square in the center of which there is a square hole and when A is a square in the center of which there is a square hole and the shape of B is the same as the shape of A and the size of B is different from the size of A . These results suggest that the coefficient $C_{AB}^{(n)}$ is factorized in a massless free scalar field in $(2+1)$ dimension. This factorization is not clear in the formal expressions in (4.7) and (4.15) and numerical calculation is important to check the factorization.

6 Conclusion and discussions

In this paper, we considered the (Rényi) mutual information, $I^{(n)}(A, B) = S_A^{(n)} + S_B^{(n)} - S_{A \cup B}^{(n)}$, of distant compact spatial regions A and B in the vacuum state of a free scalar field. The distance r between A and B is much greater than their sizes $R_{A,B}$ and the (Rényi) mutual information behaves as $I^{(n)}(A, B) \sim C_{AB}^{(n)} \langle 0 | \phi(r) \phi(0) | 0 \rangle^2$. We obtained the direct expression of $C_{AB}^{(n)}$ for arbitrary regions A and B . We performed the analytical continuation of n and obtain the mutual information $I(A, B) = \lim_{n \rightarrow 1} I^{(n)}(A, B)$. When $n = 2, 3$, $C_{AB}^{(n)}$ is not entangled, i.e. it is a simple product of functions each of which is determined by the shape of $A(B)$. For general n , $C_{AB}^{(n)}$ is not a simple product of functions each of which is determined by the shape of $A(B)$ and $C_{AB}^{(n)}$ is entangled. For example, $C_{AB}^{(n)}$ is entangled when $n = 1, 4$.

We applied our method to a massless free scalar field in $(d+1)$ dimension and performed numerical calculation for $d = 2, 3$. We showed that our method reproduce the results computed by conventional real time formalism. We showed that $C_{AB}^{(n)}$ is factorized in a $(d+1)$ -dimensional massless free scalar field by numerical calculation for $d = 2, 3$. This factorization is not clear in the formal expressions in (4.7) and (4.15) and numerical calculation is important to check the factorization.

The direct expression is useful for the numerical computation. By using the direct expression, we can compute directly $I(A, B)$ without computing S_A, S_B and $S_{A \cup B}$ respectively, so it reduces significantly the amount of computation.

It is an interesting future problem to apply our direct expression to study the shape dependence of $C_{AB}^{(n)}$. For example, the corner contribution to mutual information in $(2+1)$ dimension is an interesting problem. The corner contributions to entanglement entropy

in (2+1) dimension are universal and have important information of the QFT [32–35], however, the corner contribution to mutual information has not been studied well. Our method is useful for studying the corner contributions of mutual information. It is also an interesting future problem to generalize our method to the entanglement negativity [36, 37].

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A Derivation of $0 \leq \lambda_i < 1$

We show that the range of the eigenvalues λ_i of Y in (3.16) is $0 \leq \lambda_i < 1$. A and D in (3.10) and (3.11) are positive definite symmetric matrices because W and W^{-1} are positive definite symmetric matrices. So, $X = (A^{-1} + D)^{-1/2}$ in (3.15) is a positive definite symmetric matrix.

In order to show that Y is a positive semidefinite matrix, we use the following identity,

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \begin{pmatrix} D & E \\ E^T & F \end{pmatrix} = \begin{pmatrix} AD + BE^T & AE + BF \\ B^T D + CE^T & B^T E + CF \end{pmatrix}. \quad (\text{A.1})$$

From (A.1), we obtain $DA - 1 = -EB^T$ and $B^T = -F^{-1}E^T A$. Thus we rewrite $D - A^{-1}$ in Y as

$$D - A^{-1} = (DA - 1)A^{-1} = -EB^T A^{-1} = EF^{-1}E^T. \quad (\text{A.2})$$

Because F^{-1} is a positive definite matrix and (A.2), $D - A^{-1}$ is a positive semidefinite matrix. Therefore, $Y = X(D - A^{-1})X$ is a positive semidefinite matrix and we obtain $0 \leq \lambda_i$.

Next we consider the upper bound of λ_i . We rewrite $1 - Y$ as

$$\begin{aligned} 1 - Y &= (A^{-1} + D)^{-1/2} [A^{-1} + D - (D - A^{-1})] (A^{-1} + D)^{-1/2} \\ &= (A^{-1} + D)^{-1/2} 2A^{-1} (A^{-1} + D)^{-1/2}. \end{aligned} \quad (\text{A.3})$$

Because A^{-1} is a positive definite matrix and (A.3), $1 - Y$ is a positive definite matrix and we obtain $\lambda_i < 1$. Therefore, we have shown $0 \leq \lambda_i < 1$.

B The calculation of $F(n, a, b)$ in (4.6)

We calculate the summation $F(n, a, b)$ in (4.6) for $0 \leq a < 1$, $0 \leq b < 1$. We expand $(1 - \cos(\frac{2\pi k}{n}))^2$ in (4.6) and rewrite $F(n, a, b)$ as

$$\begin{aligned} F(n, a, b) &= \frac{n}{ab} + \frac{1}{a} \left(1 - \frac{1}{b}\right) \sum_{k=0}^{n-1} \frac{1}{1 - b \cos(\frac{2\pi k}{n})} + \frac{1}{b} \left(1 - \frac{1}{a}\right) \sum_{k=0}^{n-1} \frac{1}{1 - a \cos(\frac{2\pi k}{n})} \\ &\quad + \left(1 - \frac{1}{a}\right) \left(1 - \frac{1}{b}\right) \sum_{k=0}^{n-1} \frac{1}{1 - a \cos(\frac{2\pi k}{n})} \frac{1}{1 - b \cos(\frac{2\pi k}{n})}. \end{aligned} \quad (\text{B.1})$$

In order to calculate the summations in (B.1), we use the following expansion,

$$\frac{1}{1 - a \cos \theta} = (1 + \rho(a)^2) \frac{1}{1 - \rho(a)e^{i\theta}} \frac{1}{1 - \rho(a)e^{-i\theta}} = (1 + \rho(a)^2) \sum_{p=0}^{\infty} \sum_{p'=0}^{\infty} \rho(a)^{p+p'} e^{i(p-p')\theta} \quad (\text{B.2})$$

where

$$\rho(a) \equiv \frac{1}{a} \left(1 - \sqrt{1 - a^2} \right), \quad (\text{B.3})$$

here $0 \leq \rho(a) < 1$ for $0 \leq a < 1$, and

$$a = \frac{2\rho(a)}{1 + \rho(a)^2}. \quad (\text{B.4})$$

The expansion (B.2) in the limit $a \rightarrow 1-$ was used in [28].

B.1 The calculation of $\sum_{k=0}^{n-1} \frac{1}{1 - a \cos(\frac{2\pi k}{n})}$

By using the expansion in (B.2), we obtain

$$\sum_{k=0}^{n-1} \frac{1}{1 - a \cos(\frac{2\pi k}{n})} = (1 + \rho(a)^2) \sum_{p=0}^{\infty} \sum_{p'=0}^{\infty} \rho(a)^{p+p'} \sum_{k=0}^{n-1} e^{i(p-p')\frac{2\pi k}{n}}. \quad (\text{B.5})$$

We split the p, p' summation into three parts,

$$\sum_{p=0}^{\infty} \sum_{p'=0}^{\infty} = \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \bigg|_{p=p'+l} + \sum_{p=0}^{\infty} \sum_{l=0}^{\infty} \bigg|_{p'=p+l} - \sum_{p=0}^{\infty} \bigg|_{p'=p}, \quad (\text{B.6})$$

where we subtracted the $p = p'$ part to avoid double counting. From (B.5) and (B.6), we obtain

$$\begin{aligned} & \sum_{p=0}^{\infty} \sum_{p'=0}^{\infty} \rho(a)^{p+p'} \sum_{k=0}^{n-1} e^{i(p-p')\frac{2\pi k}{n}} \\ &= \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \rho^{2p'+l} \sum_{k=0}^{n-1} e^{il\frac{2\pi k}{n}} + \sum_{p=0}^{\infty} \sum_{l=0}^{\infty} \rho^{2p+l} \sum_{k=0}^{n-1} e^{-il\frac{2\pi k}{n}} - \sum_{p=0}^{\infty} \rho^{2p} \sum_{k=0}^{n-1} 1 \\ &= n \sum_{p'=0}^{\infty} \sum_{j=0}^{\infty} \rho^{2p'+nj} + n \sum_{p=0}^{\infty} \sum_{j=0}^{\infty} \rho^{2p+nj} - n \sum_{p=0}^{\infty} \rho^{2p} \\ &= \frac{2n}{(1 - \rho^2)(1 - \rho^n)} - \frac{n}{1 - \rho^2} = \frac{n}{1 - \rho^2} \cdot \frac{1 + \rho^n}{1 - \rho^n} \end{aligned} \quad (\text{B.7})$$

where we have used

$$\sum_{k=0}^{n-1} e^{il\frac{2\pi k}{n}} = n\delta_{l,nj} \quad (j = 0, 1, 2, \dots). \quad (\text{B.8})$$

We substitute (B.7) into (B.5) and obtain

$$\sum_{k=0}^{n-1} \frac{1}{1 - a \cos(\frac{2\pi k}{n})} = (1 + \rho(a)^2) \frac{n}{1 - \rho(a)^2} \cdot \frac{1 + \rho(a)^n}{1 - \rho(a)^n}. \quad (\text{B.9})$$

B.2 The calculation of $\sum_{k=0}^{n-1} \frac{1}{1-a \cos(\frac{2\pi k}{n})} \frac{1}{1-b \cos(\frac{2\pi k}{n})}$

In the same way as above, by using the expansion in (B.2), we obtain

$$\begin{aligned} & \sum_{k=0}^{n-1} \frac{1}{1-a \cos(\frac{2\pi k}{n})} \frac{1}{1-b \cos(\frac{2\pi k}{n})} \\ &= (1+\rho(a)^2)(1+\rho(b)^2) \sum_{k=0}^{n-1} \sum_{p=0}^{\infty} \sum_{p'=0}^{\infty} \rho(a)^{p+p'} e^{i(p-p')\frac{2\pi k}{n}} \sum_{q=0}^{\infty} \sum_{q'=0}^{\infty} \rho(b)^{q+q'} e^{i(q-q')\frac{2\pi k}{n}}. \end{aligned} \quad (\text{B.10})$$

From (B.6), we can rewrite the summations in (B.10) as

$$\begin{aligned} \sum_{p=0}^{\infty} \sum_{p'=0}^{\infty} \sum_{q=0}^{\infty} \sum_{q'=0}^{\infty} &= \left(\sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \left| \begin{array}{c} \infty \\ p'=p'+l \end{array} \right| + \sum_{p=0}^{\infty} \sum_{l=0}^{\infty} \left| \begin{array}{c} \infty \\ p'=p+l \end{array} \right| - \sum_{p=0}^{\infty} \left| \begin{array}{c} \infty \\ p'=p \end{array} \right| \right) \\ &\times \left(\sum_{q'=0}^{\infty} \sum_{m=0}^{\infty} \left| \begin{array}{c} \infty \\ q'=q'+m \end{array} \right| + \sum_{q=0}^{\infty} \sum_{m=0}^{\infty} \left| \begin{array}{c} \infty \\ q'=q+m \end{array} \right| - \sum_{q=0}^{\infty} \left| \begin{array}{c} \infty \\ q'=q \end{array} \right| \right). \end{aligned} \quad (\text{B.11})$$

We substitute (B.11) into (B.10) and obtain

$$\begin{aligned} & \frac{1}{(1+\rho(a)^2)(1+\rho(b)^2)} \sum_{k=0}^{n-1} \frac{1}{1-a \cos(\frac{2\pi k}{n})} \frac{1}{1-b \cos(\frac{2\pi k}{n})} \\ &= \sum_{k=0}^{n-1} \left[2 \left(\sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \sum_{q'=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^{2p'+l} \rho(b)^{2q'+m} e^{i(l+m)2\pi k/n} \right. \right. \\ & \quad + \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \sum_{q=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^{2p'+l} \rho(b)^{2q+m} e^{i(l-m)2\pi k/n} \\ & \quad - \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \sum_{q=0}^{\infty} \rho(a)^{2p'+l} \rho(b)^{2q} e^{il2\pi k/n} \\ & \quad \left. - \sum_{p=0}^{\infty} \sum_{q'=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^{2p} \rho(b)^{2q'+m} e^{im2\pi k/n} \right) \\ & \quad \left. + \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \rho(a)^{2p} \rho(b)^{2q} \right]. \end{aligned} \quad (\text{B.12})$$

The last term in (B.12) can be evaluated as

$$\sum_{k=0}^{n-1} \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \rho(a)^{2p} \rho(b)^{2q} = n \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2}. \quad (\text{B.13})$$

The third term in (B.12) can be evaluated as

$$\begin{aligned} \sum_{k=0}^{n-1} \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \sum_{q=0}^{\infty} \rho(a)^{2p'+l} \rho(b)^{2q} e^{il2\pi k/n} &= n \sum_{p'=0}^{\infty} \sum_{j=0}^{\infty} \sum_{q=0}^{\infty} \rho(a)^{2p'+nj} \rho(b)^{2q} \\ &= n \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(a)^n} \frac{1}{1-\rho(b)^2}. \end{aligned} \quad (\text{B.14})$$

The fourth term in (B.12) is obtained by interchanging a and b in the third term in (B.12).

We perform the p' and q summations in the second term in (B.12) and obtain

$$\begin{aligned} & \sum_{k=0}^{n-1} \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \sum_{q=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^{2p'+l} \rho(b)^{2q+m} e^{i(l-m)2\pi k/n} \\ &= \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \sum_{k=0}^{n-1} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^l \rho(b)^m e^{i(l-m)2\pi k/n}. \end{aligned} \quad (\text{B.15})$$

By using (B.6), we obtain

$$\begin{aligned} & \sum_{k=0}^{n-1} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^l \rho(b)^m e^{i(l-m)2\pi k/n} \\ &= \sum_{k=0}^{n-1} \left[\sum_{l=0}^{\infty} \sum_{\alpha=0}^{\infty} \rho(a)^l \rho(b)^{l+\alpha} e^{-i\alpha 2\pi k/n} + \sum_{m=0}^{\infty} \sum_{\alpha=0}^{\infty} \rho(a)^{m+\alpha} \rho(b)^m e^{i\alpha 2\pi k/n} - \sum_{l=0}^{\infty} \rho(a)^l \rho(b)^l \right] \\ &= n \sum_{l=0}^{\infty} \sum_{j=0}^{\infty} \rho(a)^l \rho(b)^{l+nj} + n \sum_{m=0}^{\infty} \sum_{j=0}^{\infty} \rho(a)^{m+nj} \rho(b)^m - n \frac{1}{1-\rho(a)\rho(b)} \\ &= \frac{n}{1-\rho(a)\rho(b)} \left[\frac{1}{1-\rho(b)^n} + \frac{1}{1-\rho(a)^n} - 1 \right]. \end{aligned} \quad (\text{B.16})$$

Thus, we substitute (B.16) into (B.15) and obtain the second term in (B.12)

$$\begin{aligned} & \sum_{k=0}^{n-1} \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \sum_{q=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^{2p'+l} \rho(b)^{2q+m} e^{i(l-m)2\pi k/n} \\ &= \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \frac{n}{1-\rho(a)\rho(b)} \left[\frac{1}{1-\rho(a)^n} + \frac{1}{1-\rho(b)^n} - 1 \right]. \end{aligned} \quad (\text{B.17})$$

We perform the p' and q' summations in the first term in (B.12) and obtain

$$\begin{aligned} & \sum_{k=0}^{n-1} \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \sum_{q'=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^{2p'+l} \rho(b)^{2q'+m} e^{i(l+m)2\pi k/n} \\ &= \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \sum_{k=0}^{n-1} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^l \rho(b)^m e^{i(l+m)2\pi k/n} \end{aligned} \quad (\text{B.18})$$

By using (B.8), we obtain

$$\begin{aligned} & \sum_{k=0}^{n-1} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^l \rho(b)^m e^{i(l+m)2\pi k/n} = n \sum_{j=0}^{\infty} \sum_{l=0}^{nj} \rho(a)^l \rho(b)^{nj-l} \\ &= n \sum_{j=0}^{\infty} \rho(b)^{nj} \left(\frac{1 - (\rho(a)/\rho(b))^{nj+1}}{1 - (\rho(a)/\rho(b))} \right) = \frac{n}{\rho(b) - \rho(a)} \left[\frac{\rho(b)}{1 - \rho(b)^n} - \frac{\rho(a)}{1 - \rho(a)^n} \right]. \end{aligned} \quad (\text{B.19})$$

We substitute (B.19) into (B.18) and obtain the first term in (B.12)

$$\begin{aligned} & \sum_{k=0}^{n-1} \sum_{p'=0}^{\infty} \sum_{l=0}^{\infty} \sum_{q'=0}^{\infty} \sum_{m=0}^{\infty} \rho(a)^{2p'+l} \rho(b)^{2q'+m} e^{i(l+m)2\pi k/n} \\ &= \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \frac{n}{\rho(b)-\rho(a)} \left[\frac{\rho(b)}{1-\rho(b)^n} - \frac{\rho(a)}{1-\rho(a)^n} \right]. \end{aligned} \quad (\text{B.20})$$

Finally, we substitute (B.13), (B.14), (B.17) and (B.20) into (B.12) and obtain

$$\begin{aligned} & \frac{1}{(1+\rho(a)^2)(1+\rho(b)^2)} \sum_{k=0}^{n-1} \frac{1}{1-a \cos\left(\frac{2\pi k}{n}\right)} \frac{1}{1-b \cos\left(\frac{2\pi k}{n}\right)} \\ &= 2 \left[\frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \frac{n}{\rho(b)-\rho(a)} \left(\frac{\rho(b)}{1-\rho(b)^n} - \frac{\rho(a)}{1-\rho(a)^n} \right) \right. \\ & \quad + \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \frac{n}{1-\rho(a)\rho(b)} \left(\frac{1}{1-\rho(a)^n} + \frac{1}{1-\rho(b)^n} - 1 \right) \\ & \quad \left. - n \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \left(\frac{1}{1-\rho(a)^n} + \frac{1}{1-\rho(b)^n} \right) \right] \\ & \quad + n \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \\ &= 2n \frac{1}{1-\rho(a)^2} \frac{1}{1-\rho(b)^2} \frac{1}{\rho(a)-\rho(b)} \frac{1}{1-\rho(a)\rho(b)} \\ & \quad \times \left[\frac{\rho(a)(1-\rho(b)^2)}{1-\rho(a)^n} - \frac{\rho(b)(1-\rho(a)^2)}{1-\rho(b)^n} - \frac{1}{2}(\rho(a)-\rho(b))(1+\rho(a)\rho(b)) \right]. \end{aligned} \quad (\text{B.21})$$

We substitute (B.9) and (B.21) into (B.1) and obtain

$$\begin{aligned} F(n, a, b) &= n \frac{(1+p^2)(1+q^2)}{4pq} \left[2 - \frac{(1-p)(1+p^n)}{(1+p)(1-p^n)} - \frac{(1-q)(1+q^n)}{(1+q)(1-q^n)} \right. \\ & \quad + \frac{2}{(1+p)(1+q)(p-q)(1-pq)} \left\{ \frac{1-p}{1-p^n} p(1-q)^2(1+q) - \frac{1-q}{1-q^n} q(1-p)^2(1+p) \right. \\ & \quad \left. \left. - (p-q)(1+pq - (p+q)pq) \right\} \right] \end{aligned} \quad (\text{B.22})$$

where $0 \leq a < 1$, $0 \leq b < 1$ and

$$p \equiv \rho(a) = \frac{1}{a} \left(1 - \sqrt{1-a^2} \right), \quad q \equiv \rho(b) = \frac{1}{b} \left(1 - \sqrt{1-b^2} \right). \quad (\text{B.23})$$

Thus (B.22) is equal to (4.7).

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