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## Modular Hamiltonian for Excited States in Conformal Field Theory

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We present a novel replica trick that computes the relative entropy of two arbitrary states in conformal field theory. Our replica trick is based on the analytic continuation of partition functions that break the  $Z_n$  replica symmetry. It provides a method for computing arbitrary matrix elements of the modular Hamiltonian corresponding to excited states in terms of correlation functions. We show that the quantum Fisher information in vacuum can be expressed in terms of two-point functions on the replica geometry. We perform sample calculations in two-dimensional conformal field theories.

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In recent years entanglement theory has found numerous applications in the study of quantum phases of matter, relativistic field theories and gravity. Most of these applications focus on an entanglement measure in bipartite pure states known as the entanglement entropy. Unfortunately, in relativistic field theories entanglement entropy suffers from ultraviolet divergences. In gauge theories the definition of entanglement entropy is ambiguous [1]. In this Letter, we present a method to compute, in field theory, another measure called relative entropy that is provably ultraviolet finite, universal, and free of gauge ambiguities [1,2].

Relative entropy is a measure of distinguishability between two states and has nice monotonicity and positivity properties. It appears naturally in the definition of entanglement measures for mixed states such as mutual information and the relative entropy of entanglement [3]. Recently, thinking in terms of relative entropy in quantum field theories coupled to gravity has led to new developments such as a proof of the quantum Bousso bound [4], and the identification of new gravitational positive energy theorems [5].

The relative entropy of the density matrix  $\phi$  with respect to  $\psi$  is defined to be

$$S(\phi \| \psi) = tr(\phi \log \phi) - tr(\phi \log \psi). \tag{1}$$

Note that relative entropy is ill-defined when  $\psi$  is pure. The relative entropy of two states can be thought of as the expectation value of the difference of the modular Hamiltonians of the two states

$$S(\phi ||\psi) = \langle \phi | H(\psi) - H(\phi) | \phi \rangle$$
  
= tr[(\phi - \psi) H(\psi)] - \Delta S. (2)

Here the positive Hermitian operator  $H(\psi) = -\log \psi$  is the modular Hamiltonian of  $\psi$ , and  $\Delta S$  is the difference of the entanglement entropies of  $\phi$  and  $\psi$ . If we formally define the *generalized free energy* function  $F_{\psi}(\phi) =$ tr $[\phi H(\psi)] - S(\phi)$ , then the relative entropy is the free energy difference between the two states

$$S(\phi \| \psi) = F_{\psi}(\phi) - F_{\psi}(\psi). \tag{3}$$

The function  $F_{\psi}$  has all the properties one expects from free energy in a thermodynamic theory where  $\psi = e^{-H(\psi)}$  plays the role of the equilibrium state [5,6]. Note that  $F_{\psi}$  achieves its minimum on the equilibrium state  $\psi$ . [This is a consequence of positivity of relative entropy:  $F_{\psi}(\phi) \ge F_{\psi}(\psi)$ ].

In this Letter, we construct a class of field theory partition functions that is proportional to  $tr(\phi\psi^{n-1})$ . Their analytic continuation provides the relative entropy and the modular Hamiltonian of density matrices in excited states  $|\phi\rangle$  and  $|\psi\rangle$  reduced to the subsystem. While the formalism presented here applies to all quantum field theories we focus on conformal field theories to have access to more computational tools.

According to the operator-state correspondence in conformal field theory (CFT) there is a one-to-one map between wave functionals and operators in the Hilbert space. In radial quantization, the wave functional of an excited state  $|\psi\rangle$  is found by performing a Euclidean path integration with the corresponding operator  $\Psi$  inserted. Restricting to subsystem A the state is described by a density matrix  $\psi_A$ ; see Fig. 1. To simplify notation we suppress the subsystem index A, and use  $\psi$  to refer to the reduced state.

In principle, one can compute the logarithm of the density matrix directly from the path integral by taking

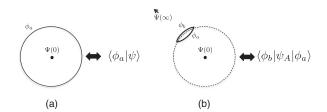


FIG. 1. (a) Operator-state correspondence in radial quantization of conformal field theories. (b) Reduced density matrix corresponds to a path integral with two operator insertions and a cut on the subsystem.

the logarithm of a path-ordered operator using the so-called Magnus expansion; however, in practice this is too hard. Here, we propose an alternative method to compute matrix elements of the modular Hamiltonian of excited states from the analytic continuation of correlation functions. Our method is a generalization of the replica trick in Refs. [7,8] to the case where one breaks the  $Z_n$  symmetry among replicas. This enables us to compute matrix elements of the modular operator for all states. This is in contrast with the old replica method which was restricted to states that have local modular Hamiltonians, the only known example of which is vacuum reduced to a half-space or spherical subsystems [9,10]. (In two-dimensional CFTs, a finite temperature state on a line also has reduced states with a local modular Hamiltonian [11]).

Relative entropy and modular Hamiltonian.—Consider the Hermitian operator  $\{\phi, \psi^{n-1}\} = \frac{1}{2}(\phi\psi^{n-1} + \psi^{n-1}\phi)$ built out of reduced density matrices  $\phi$  and  $\psi$  corresponding to global states  $|\phi\rangle$  and  $|\psi\rangle$ , respectively. Its trace in conformal field theory corresponds to the *n*-sheeted partition function tr $(\phi\psi^{n-1})$ . The idea is to take advantage of the analytic properties of correlators by using the operator identity

$$\operatorname{tr}(\phi \log \psi) = \partial_n(\phi \psi^{n-1}) \Big|_{n \to 1}.$$
 (4)

Our partition functions of interest, tr( $\phi \psi^{n-1}$ ), break the  $Z_n$  replica symmetry present in both the Renyi entropy and Renyi relative entropy replica tricks [8,12]. In contrast with the symmetric case, our partition functions are not monotonic in index *n*, and have no known operational interpretations. Nonetheless, under the assumption of analyticity, they provide a computational tool for finding relative entropies and the diagonal elements of the modular Hamiltonian of excited states

$$S(\phi \| \psi) = \partial_n \log \left[ \frac{\operatorname{tr}(\phi^n) \operatorname{tr}(\psi)^{n-1}}{\operatorname{tr}(\phi \psi^{n-1}) \operatorname{tr}(\phi)^{n-1}} \right]_{n \to 1}$$
$$\langle \phi | H(\psi) - H(\sigma_0) | \phi \rangle = \log \left[ \frac{\langle \phi | \sigma_0^{n-1} | \phi \rangle \operatorname{tr}(\psi)^{n-1}}{\langle \phi | \psi^{n-1} | \phi \rangle \operatorname{tr}(\sigma_0)^{n-1}} \right]_{n \to 1}, \quad (5)$$

where  $\sigma_0$  is the reduced density matrix in vacuum. We subtract the vacuum modular Hamiltonian so that we have ultraviolet finite quantities at any *n*. The off-diagonal elements of the modular Hamiltonian are obtained from its diagonal element in superposition states; see Supplemental Material [13].

Each of the terms inside the logarithm above can be expressed as a Euclidean path integration with operator insertions on a replicated or the original geometry [14]. For instance, consider the terms tr( $\rho\psi^{n-1}$ ). Sewing *n* copies of the density matrix cyclically along the boundary of their subsystems we obtain *n*-sheeted replica manifold  $\mathcal{R}_n$  and 2n operator insertions (Fig. 2)

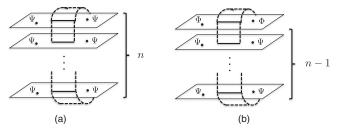


FIG. 2. (a) Entanglement entropy replica trick: the Euclidean path integration on the *n*-sheeted manifold corresponding to the partition function  $tr(\psi^n)$ . (b) The  $Z_n$ -breaking partition  $tr(\phi\psi^{n-1})$  that appears in our relative entropy replica trick.

$$\operatorname{tr}(\phi\psi^{n-1}) = Z(\mathcal{R}_n) \langle \Phi(z'_n) \Phi(z_n) \mathcal{O}_{\Psi}^{(n-1)} \rangle_{\mathcal{R}_n}$$
$$\mathcal{O}_{\Phi}^{(m)} = \prod_{i=1}^m \Phi(z'_i) \Phi(z_i) \tag{6}$$

where  $z_i$  and  $z'_i$  are points z and z' on the *i*th sheet of  $\mathcal{R}_n$ . It is important to note that plugging Eq. (6) into Eq. (5) all partition function terms cancel and we are left only with correlation functions at any n which are free of ultraviolet divergences.

Written explicitly in terms of correlation functions we find the main results of this section:

 $S(\phi \| \psi)$ 

$$= \partial_n \log \left[ \frac{\langle \mathcal{O}_{\Phi}^{(n)} \rangle_{\mathcal{R}_n} \langle \Psi(z_1') \Psi(z_1) \rangle_{\mathcal{R}_1}^{n-1}}{\langle \Phi(z_n') \Phi(z_n) \mathcal{O}_{\Psi}^{(n-1)} \rangle_{\mathcal{R}_n} \langle \Phi(z_1') \Phi(z_1) \rangle_{\mathcal{R}_1}^{n-1}} \right]_{n \to 1}$$
  
$$\langle \phi | H(\psi) - H(\sigma_0) | \phi \rangle$$
  
$$= \partial_n \log \left[ \frac{\langle \Phi(z_n') \Phi(z_n) \rangle_{\mathcal{R}_n} \langle \Psi(z_1') \Psi(z_1) \rangle_{\mathcal{R}_1}^{n-1}}{\langle \Phi(z_n') \Phi(z_n) \mathcal{O}_{\Psi}^{(n-1)} \rangle_{\mathcal{R}_n}} \right]_{n \to 1}$$
  
$$\langle \chi | H(\psi) - H(\sigma_0) | \phi \rangle = \partial_n \left[ \log \left[ \frac{X_{-1}}{X_{+1}} \right] + i \log \left[ \frac{X_{-i}}{X_{+i}} \right] \right]_{n \to 1}$$

where

$$X_{c} = E_{\Phi\Phi}(\mathcal{O}_{\Psi}^{(n-1)}) + |c|^{2}E_{\chi\chi}(\mathcal{O}_{\Psi}^{(n-1)}) + cE_{\Phi\chi}(\mathcal{O}_{\Psi}^{(n-1)}) + \text{H.c.} E_{\Phi\chi}(\mathcal{O}) = \frac{\langle \Phi(z'_{n})\chi(z_{n})\mathcal{O}\rangle_{\mathcal{R}_{n}}}{\sqrt{\langle \Phi(z'_{1})\Phi(z_{1})\rangle_{\mathcal{R}_{1}}\langle \chi(z'_{1})\chi(z_{1})\rangle_{\mathcal{R}_{1}}}}$$
(7)

Here, we have assumed that  $\langle \psi | \phi \rangle = 0$ .

Quantum Fisher information.—Our replica trick connects the modular Hamiltonian of excited states to analytic continuation of 2n-point correlation functions. Apart from integrable models and large central charge theories, obtaining analytic expressions for 2n-point functions is an intractable problem. However, as we show in this section a great simplification occurs once we focus on near-vacuum states.

Let us first consider a one-parameter family of states  $(|\phi\rangle + \epsilon |X\rangle)/\sqrt{1 + \epsilon^2}$  perturbed around  $|\phi\rangle$  in perpendicular direction  $|X\rangle$ . The reduced density matrix on subsystem *A* expanded in  $\epsilon$  has the form

$$\phi + \epsilon \rho_X^{(1)} + \epsilon^2 \rho_X^{(2)} + O(x^3).$$

Relative entropy is a smooth nondegenerate function of two states. Hence, the relative entropy of two nearby states expanded in  $\epsilon$  vanishes to the first order. The coefficient of the second order term,  $F_{\phi}(X, Y)$ , is called the quantum Fisher information at point  $\phi$  in the space of density matrices:

$$S(\phi + \epsilon \rho_X \| \phi) = \epsilon^2 F_{\phi}(X, X) + O(\epsilon^3).$$

This function defines a metric on the space of perturbations to state  $\phi$ 

$$2F_\phi(X,Y)=F_\phi(X+Y,X+Y)-F_\phi(X,X)-F_\phi(Y,Y).$$

Quantum Fisher information is a local measure of distinguishability, and is intimately connected with uncertainty relations [15]. Consider the relative entropy of two nearby states. Our replica trick in Eq. (5) implies

$$F_{\phi}(X,X) = \partial_{n} \left[ n \sum_{m=0}^{n-2} \frac{\langle \{X,\Phi\} \Phi^{2m} \{X,\Phi\} \Phi^{2(n-m-2)} \rangle_{\mathcal{R}_{n}} \langle \Phi \Phi \rangle_{\mathcal{R}_{1}}}{\langle \Phi^{2n} \rangle_{\mathcal{R}_{n}} \langle XX \rangle_{\mathcal{R}_{1}}} \right]_{n \to 1}$$

$$(8)$$

where X and  $\Phi$  denote the operators that create the perturbations corresponding to  $|X\rangle$  and  $|\phi\rangle$ , respectively. The location of operator insertions are the same as Eq. (6).

For near vacuum states, we replace  $\Phi$  in Eq. (8) with the identity. The quantum Fisher information takes the form of an analytic continuation of two-point functions on the replica geometry; see Fig. 3:

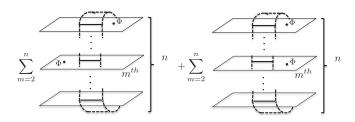


FIG. 3. The type of two-point functions on the replica manifold whose analytic continuation determines quantum Fisher information in vacuum.

$$F_{\sigma}(X,X) = \partial_{n} \left[ \sum_{z^{\pm}=z,z'} K_{X}(z^{+},z^{-}) \right]_{n \to 1}$$
$$K_{X}(z^{+},z^{-}) = n \sum_{m=1}^{n-1} \frac{\langle X(z_{1}^{+})X(z_{m+1}^{-}) \rangle_{\mathcal{R}_{n}}}{\langle X(z_{0})X(z_{0}') \rangle_{\mathcal{R}_{1}}}.$$
(9)

This implies that in arbitrary dimensions the vacuum Fisher information of any primary excitation reduced to a ball or radius R is universal in the sense that it depends only on energy and subsystem size. In the remainder of this Letter, we provide examples of relative entropies, modular Hamiltonians, and quantum Fisher information in two-dimensional CFTs computed using the method above.

Examples in two dimensions.-Relative entropy of excited states: Consider a free massless boson CFT in two dimensions on a circle of radius R and a subsystem at A = (-l/2, l/2). We are interested in the excited states obtained by the action of chiral vertex operators on vacuum at past infinity:  $|\alpha\rangle = V_{\alpha}|\Omega\rangle = e^{i\alpha\phi}|\Omega\rangle$ , where  $\phi$  is the boson field. The dimension of this operator is  $(h, \bar{h}) =$  $(\alpha^2/2, 0)$ . Here x = l/R is the dimensionless parameter. In the Supplemental Material [13] it is shown that in two dimensions one can equally use correlators on a cylinder, full complex plane, or a strip in our formulae in Eq. (7) for relative entropy and modular Hamiltonian. The conformal factors found from the change of coordinates vanish in the limit of  $n \rightarrow 1$ . In a free theory with a nondegenerate ground state all correlation functions are determined by Wick's theorem [16]:

$$\langle V_{-\alpha} \mathcal{O}_{\beta}^{(n-1)} V_{\alpha} \rangle_{S} = [2 \sin(\pi x/n)]^{\beta^{2}(1-n)-\alpha^{2}} g_{n}^{-(n-2)\beta^{2}-2\alpha\beta}$$

where *S* refers to correlators on a strip of width  $2\pi$ , and  $g_n = \sin(\pi x)/n \sin(\pi x/n)$ . For holomorphic excitations  $[V_{\alpha}]^{\dagger} \sim V_{-\alpha}$ . Therefore,

$$S(\alpha \| \beta) = \partial_n \log \left( \frac{\langle \mathcal{O}_{\alpha}^{(n)} \rangle_S \langle V_{-\beta} V_{\beta} \rangle_S^{n-1}}{\langle V_{-\alpha} V_{\alpha} \mathcal{O}_{\beta}^{(n-1)} \rangle_S \langle V_{-\alpha} V_{\alpha} \rangle_S^{n-1}} \right)$$
$$= (\alpha - \beta)^2 [1 - \pi x \cot(\pi x)]. \tag{10}$$

The analytic continuation used above is justified in the Supplemental Material [13]. When  $\beta = 0$  this matches the result previously found using a  $Z_n$ -symmetric replica trick in Ref. [12]:  $S(\alpha || 0) = \alpha^2 [1 - \pi x \cot(\pi x)]$ . Interestingly, the answer in Eq. (5) is symmetric in its arguments,  $S(\alpha || \beta) = S(\beta || \alpha)$ . These excited states further have the property that  $S(\alpha) = S(\beta) = S(\sigma_0)$ , where  $\sigma_0$  is the vacuum density matrix. Hence, we find  $tr(\rho_\alpha H_\beta) = tr(\rho_\beta H_\alpha)$  for all  $\alpha$  and  $\beta$ .

Modular Hamiltonian of excited states: In the free c = 1 CFT, Wick contractions imply that a correlator is zero unless  $\sum_i \alpha_i = 0$ . For all  $\alpha \neq \gamma$  we have

 $\langle V_{-\alpha}V_{\gamma}\mathcal{O}_{\beta}^{(n-1)}\rangle_{S} = 0$ . As a result,  $X_{c}$  in Eq. (7) is independent of c, and we find that the modular operator  $H_{\beta}$  has no off-diagonal terms in the  $|\alpha\rangle$  basis.

The diagonal elements are

$$\langle \alpha | H(\beta) - H(\sigma_0) | \alpha \rangle = \beta (\beta - 2\alpha) [1 - \pi x \cot(\pi x)].$$

Note that in the limit  $\alpha = \beta$  this reproduces  $-\beta^2 [1 - \pi \cot(\pi x)] = -S(\beta | \sigma_0)$  as it should. In the limit  $\beta = 0$  the difference of modular Hamiltonians is the zero operator and hence the answer should vanish as it does.

Quantum Fisher metric around the vacuum: Consider an arbitrary two-dimensional conformal field theory on a circle. The vacuum Fisher information is given by Eq. (9). After some algebra we find

$$F_{\sigma}(X,X) = \partial_n [2s_n(0) + s_n(x) + s_n(-x)]_{n \to 1}$$
$$s_n(x) = \left(\frac{\sin^2(\pi x)}{n^2}\right)^{h+\bar{h}} n \sum_{m=1}^{n-1} \sin\left[\pi(m+x)/n\right]^{-2(h+\bar{h})}.$$

For simplicity we expand in small x to find

$$F_{\sigma} \simeq \partial_{n} \left[ 4 \left( \frac{\pi x}{n} \right)^{2(h+\bar{h})} n \sum_{m=1}^{n-1} \sin(\pi m/n)^{-2(h+\bar{h})} \right]_{n \to 1}$$
$$= \frac{2(\pi x)^{2(h+\bar{h})} \sqrt{\pi} \Gamma(h+\bar{h}+1)}{\Gamma(h+\bar{h}+\frac{3}{2})}, \qquad (11)$$

where we have used the analytic continuation found in Ref. [17].

Multiple intervals: The replica trick developed here can be applied to subsystems with multiple intervals. As an example we focus on mutual information in vacuum

$$S(\sigma_{AB} \| \sigma_A \otimes \sigma_B) = I(A : B), \tag{12}$$

where *A* and *B* are nonoverlapping intervals. According to Eq. (5), the relative entropy is the analytic continuation of the vacuum partition functions on manifolds  $Z_n^{AB}$  and  $Z_n^{A,B}$  illustrated in Fig. 4

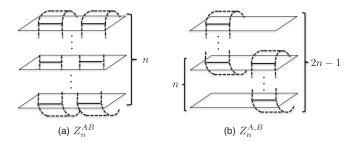


FIG. 4. (a) The *n*-sheeted manifold corresponding to the partition function  $Z_n^{AB}$ . (b) The  $Z_n$ -breaking partition  $Z_n^{A,B} = \text{tr}[\sigma_{AB}(\sigma_A \otimes \sigma_B)^{\otimes n-1}]$ .

$$I(A:B) = \lim_{n \to 1} \frac{1}{n-1} (\log Z_n^{AB} - \log Z_n^{A,B}).$$
(13)

The first partition function  $Z_n^{AB}$  corresponds to Renyi entropies of  $\sigma_{AB}$ . Therefore, from Eq. (12) all we need to check is

$$\partial_n Z_n^{A,B} \Big|_{n \to 1} = S(A) + S(B).$$
<sup>(14)</sup>

The Riemann-Hurwitz formula tells us that  $Z_n^{AB}$  has genus (n-1) and  $Z_n^{A,B}$  is simply the Riemann sphere. Following Ref. [18] we compute the path integral over these manifolds using twist operators in an orbifold theory with replica copies of the fields. In particular, up to normalization  $Z_n^{A,B}$  is the correlation function

$$\langle \sigma_{(1\cdots n)}(u_A)\sigma_{(n\cdots 1)}(v_A)\sigma_{(n\cdots 2n-1)}(u_B)\sigma_{(2n-1\cdots n)}(v_B)\rangle$$

in a (2n-1) replica theory. Here  $u_A$  and  $v_A$  are the endpoints of interval A, and going around the twist operator  $\sigma_{(1\cdots m)}$  the replica fields transform as  $(X^1, X^2 \cdots X^m, X^{m+1} \cdots X^{2n-1}) \rightarrow (X^2, \cdots X^m, X^1, X^{m+1} \cdots X^{2n-1})$ . Inserting a resolution of the identity on the *n*th sheet splits the correlator into a sum over the product of sphere one-point functions. (see Fig. 5). The sphere one-point function is zero unless  $\Phi_k$  is the identity operator. In other words,

$$S_n^{A,B} = S_n^A + S_n^B \tag{15}$$

which is the sum of Renyi entropies of intervals A and B, and hence Eq. (14) follows.

*Discussion.*—In this Letter, we have developed a replica trick that takes advantage of breaking the replica symmetry to access the modular Hamiltonian of excited states. In the absence of the  $Z_n$  replica symmetry Renyi entropies are not monotonic in n; hence, our method cannot be used to obtain lower or upper bounds on relative entropy. The applicability of this method crucially relies on our ability to analytically continue correlation functions in n. According to the Carlson theorem [19], in order to find the unique analytic continuation of Renyis at integer n one needs to further fix the behavior at  $n \to \pm i\infty$ . We postpone a careful study of this asymptotic choice and its physical implications to future work.

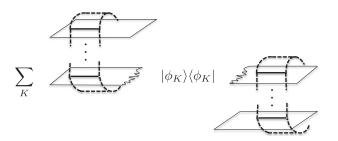


FIG. 5. Inserting the resolution of the identity in  $Z_n^{AB}$ , we observe that at each K we multiply sphere one-point functions that are zero unless  $\Phi_K$  is the identity.

The correlation functions needed to compute the modular operator of an excited state are 2n-point functions. There are not many examples of CFTs for which we have access to high-point correlators. One class of such CFTs is free theories which we briefly discussed. Another class is CFTs with large central charge, where one can reduce the calculation of *n*-point functions of heavy operators to a classical monodromy problem for differential equations that correlation functions satisfy [20].

In holographic theories, the vacuum Fisher information in spherical subsystems was recently shown to be dual to canonical energy in gravity [21]. This confirms the universal feature suggested by Eq. (9). It would be interesting to understand the connection between the CFT calculation of this quantity and canonical energy in the bulk.

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