Letter

Efficient simulation of low-temperature physics in one-dimensional gapless systems

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We discuss the computational efficiency of the finite-temperature simulation with minimally entangled typical thermal states (METTS). To argue that METTS can be efficiently represented as matrix product states, we present an analytic upper bound for the average entanglement Rényi entropy of METTS for a Rényi index $0 < q \leqslant 1$. In particular, for one-dimensional (1D) gapless systems described by conformal field theories, the upper bound scales as $O(cN^0 \log \beta)$ where c is the central charge and N is the system size. Furthermore, we numerically find that the average Rényi entropy exhibits a universal behavior characterized by the central charge and is roughly given by half of the analytic upper bound. Based on these results, we show that METTS can provide a speedup compared to employing the purification method to analyze thermal equilibrium states at low temperatures in 1D gapless systems.

Introduction. Simulating quantum many-body systems at finite temperature is an everlasting topic in statistical physics and computational physics. While thermal equilibrium states at inverse temperature β of a quantum system with Hamiltonian H can be described by the canonical Gibbs state

$$\rho_\beta^{(\mathrm{can})} \equiv \frac{e^{-\beta H}}{\mathrm{Tr}(e^{-\beta H})}, \tag{1}$$

the computational cost to construct it directly diverges exponentially with system size, which makes it unrealistic in practice to be accurately prepared.

The minimally entangled typical thermal states (METTS) algorithm [1,2] is one of the methods developed to efficiently simulate finite-temperature quantum systems. Considering a spin-$1/2$ chain of length N, the orthogonal 2^N classical product states $|P_i\rangle = \otimes_{\mathrm{sites}\ n} |i_n\rangle$ form a complete basis of the whole Hilbert space, where $\{|i_n\rangle\}$ is an orthogonal basis of each site. METTS are a class of states defined as

$$|\mu_i\rangle = \frac{e^{-\beta H/2} |P_i\rangle}{\sqrt{\langle P_i | e^{-\beta H} | P_i \rangle}}. \tag{2}$$

By construction, $\rho_\beta^{(\mathrm{can})}$ can be decomposed as a classical mixture of METTS,

$$\rho_\beta^{(\mathrm{can})} = \sum_i p_i |\mu_i\rangle\langle\mu_i|, \quad p_i \equiv \frac{\langle P_i | e^{-\beta H} | P_i \rangle}{\sum_j \langle P_j | e^{-\beta H} | P_j \rangle}. \tag{3}$$

To recover $\rho_\beta^{(\mathrm{can})}$ accurately, one may sum over 2^N METTS with weight p_i, but performing such a calculation is usually intractable. However, the METTS algorithm [1,2] enables one

to generate a Markov chain of METTS and sample METTS according to the probability distribution p_i. Thus, there is no need to calculate p_i, and one can automatically sample only METTS with large p_i. Empirically, it is known that one only needs to sample roughly 10–100 METTS to get accurate enough thermal expectation values of local observables. As a result, the most computationally costly part of this algorithm is to prepare each METTS by the imaginary-time evolution of the product state. As evaluated in Refs. [1,2], the computation time to prepare a METTS with a matrix product state (MPS) ansatz [3] scales as $ND^3\beta$, where D is the bond dimension of the MPS.

The METTS algorithm is indeed very efficient for simulating low-temperature physics in one-dimensional (1D) gapped systems because it is expected that D can be upper bounded by the bond dimension necessary to approximate the ground state [1,2], which does not scale with N or β [4,5].

On the other hand, how well METTS behaves in 1D gapless systems is not clear at low temperature, while at high enough temperature it is expected to be similarly efficient to gapped systems. There are many reasons for this. First, the arguments presented for gapped systems do not apply to gapless systems. At the low-temperature limit, METTS converge to the ground state, whose entanglement scales as $\mathcal{O}(\log N)$ for a half of the whole 1D gapless system. This implies that D can be upper bounded by a polynomial of N, which does not manifest the efficiency of METTS when N is large. Therefore, one needs to understand how entanglement grows under imaginary-time evolution for a generic METTS [6].

Can we give a bound of entanglement growth under imaginary-time evolution for generic METTS? Is METTS efficient for simulating low-temperature physics of 1D gapless systems? To answer these questions, we focus on 1D gapless

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systems whose low-energy sectors are well described by 2D conformal field theories (CFTs). After presenting some hints from CFT analyses, we prove that for the Rényi index $0 < q \leqslant 1$, the average entanglement Rényi entropy of a METTS decomposition is upper bounded by that of the thermofield double (TFD) state. Furthermore, we numerically show that the average entanglement Rényi entropy is about half of the analytic upper bound. Based on these results, we evaluate the bond dimension required to approximate METTS and the computation time for generating METTS. In the end, we demonstrate the superiority of the METTS algorithm over the TFD algorithm [7,8] (also called the ancilla method or purification method) at low temperatures in 1D gapless systems.

Hints from CFT computation. While it is difficult to analytically compute Rényi entropies for all the METTS, we can do it for a special class of METTS with a boundary conformal field theory (BCFT) computation. A BCFT is a CFT defined on a manifold with boundaries whose boundary conditions maximally preserve the conformal symmetries. Such boundary conditions, when regarded as quantum states, are called boundary states. One crucial feature of boundary states is that they are product states [9]. Therefore, for a boundary state $|B\rangle$, $e^{-\beta H/2}|B\rangle$ turns out to be a METTS.

For simplicity, let us consider a 1D system defined on an infinite line. The density matrix $e^{-\beta H/2}|B\rangle\langle B|e^{-\beta H/2}$ is realized by considering a path integral of an infinite strip with width β. The qth entanglement Rényi entropy [10] of a half line A can be computed by evaluating the expectation value of a so-called twist operator inserted at the center of the strip [11,12] and turns out to be

$$S_A^{(q)} = \frac{c}{12}\left(1 + \frac{1}{q}\right)\log\left(\frac{2\beta}{\pi\epsilon}\right) + \text{const}, \qquad (4)$$

where c is the CFT central charge, and ϵ is the UV cutoff. The constant term does not depend on q but on the details of $|B\rangle$. Note that, except for this constant part, the above result is universal for any CFT and any $|B\rangle$. Also note that c roughly counts the degrees of freedom included in the CFT. For example, a free boson CFT has $c = 1$ and an n-copy of free-boson CFTs has $c = n$.

From this result, one may expect that the average Rényi entropy of METTS has a similar scaling. With these as hints, let us move on to rigorous analyses.

Analytic upper bound. From now on, we will present a theorem which provides a rigorous upper bound for the average Rényi entropy of a METTS decomposition.

We will utilize the TFD state. Consider two identical copies L and R of the original system ($\mathcal{H} \cong \mathcal{H}_L \cong \mathcal{H}_R$). Let $\mathcal{T}$ be an antiunitary operator that commutes with the Hamiltonian H. Then the TFD state $|\text{TFD}\rangle \in \mathcal{H}_L \otimes \mathcal{H}_R$ is defined as

$$|\text{TFD}\rangle = \sum_n e^{-\beta E_n/2} |n\rangle_L \otimes |\bar{n}\rangle_R, \qquad (5)$$

where $|n\rangle$ are eigenstates of H with energy E_n and $|\overline{\psi}\rangle_R = \mathcal{T}|\psi\rangle_L$. Since classical product states $\{|P_i\rangle\}_i$ form a complete orthonormal basis of $\mathcal{H}$, we have

$$|\text{TFD}\rangle = (e^{-\beta H/2} \otimes I_R) \sum_i |P_i\rangle_L \otimes |\overline{P_i}\rangle_R. \qquad (6)$$

The TFD state is a (symmetric) purification of the canonical Gibbs state, i.e., $\rho_\beta^{(\text{can})} \propto \text{Tr}_R[|\text{TFD}\rangle\langle\text{TFD}|]$. Therefore, one can also simulate finite-temperature quantum systems with TFD states. Dividing the original system into A and its complement B, then each of the two copies L and R contains a copy of A. We label them A_L and A_R, respectively.

We find that the average entanglement Rényi entropy of A over METTS is upper bounded by the entanglement Rényi entropy of $A_L A_R$ in $|\text{TFD}\rangle$ associated with the same β, for a Rényi index $0 < q \leqslant 1$.

Theorem 1. For $0 < q \leqslant 1$, there holds

$$\overline{S_A^{(q)}} \equiv \sum_i p_i S_A^{(q)}(|\mu_i\rangle) \leqslant S_{A_L A_R}^{(q)}(|\text{TFD}\rangle), \qquad (7)$$

if $|\overline{P_i}\rangle_R$ are product states for A_R and B_R.

For generic quantum many-body systems, it is plausible to expect that $|\overline{P_i}\rangle \equiv \mathcal{T}|P_i\rangle$ is also a product state. For the models presented in this Letter, $\mathcal{T}$ is simply the complex conjugate with respect to the spin basis, and this condition is satisfied.

A detailed proof is presented in the Supplemental Material [13], which utilizes the concavity of $S^{(q)}$ for $0 < q \leqslant 1$ since we used the concavity of $S^{(q)}$. This also means our proof is not valid for $q > 1$. However, we numerically find that the upper bound (7) is valid even for $q > 1$ in all the examples we study in this Letter. It will be interesting to answer whether the result (7) is valid for $q > 1$ in general.

In fact, the $q = 1$ case of this theorem follows directly from Theorem 7 of Ref. [14], which was considered in a different context related to black hole physics. However, the extension to $0 < q < 1$ is necessary and sufficient to evaluate the required bond dimensions for an MPS to approximate METTS.

Let us then go back to 1D gapless systems defined on an infinite line and take the subsystem A as a half of it. With CFT computations (see, e.g., Ref. [15]), one finds

$$\overline{S_A^{(q)}} \leqslant S_{A_L A_R}^{(q)}(|\text{TFD}\rangle) = \frac{c}{6}\left(1 + \frac{1}{q}\right)\log\left(\frac{\beta}{\pi\epsilon}\right), \qquad (8)$$

for any CFT. This rigorous upper bound turns out to be twice the right-hand side of (4) at leading order.

Numerical study in spin systems. After obtaining the rigorous bound (8), let us numerically study the average entanglement Rényi entropy of METTS in specific models. Our results show that it exhibits a universal behavior characterized only by the central charge of the associated CFT, similar to (4) for a regularized boundary state.

Numerical simulations are performed for two models with different central charges, symmetries, and integrabilities. We take the spin quantization axis along the ν direction ($\nu = x, y, z$) and choose eigenvectors of S_n^ν as $\{|i_n\rangle\}$ (which appears in the definition of $|P_i\rangle$). Here, $S_n^{x,y,z}$ are the spin operators associated to the site n.

The first model is the transverse-field Ising chain (TFI) with the open boundary condition,

$$H = -\sum_{n=1}^{N-1} S_n^z S_{n+1}^z - \gamma \sum_{n=1}^{N} S_n^x, \qquad (9)$$

which is integrable. We set $\gamma = 1/2$ so that the model is critical [11,16]. This theory is well described by CFT with a
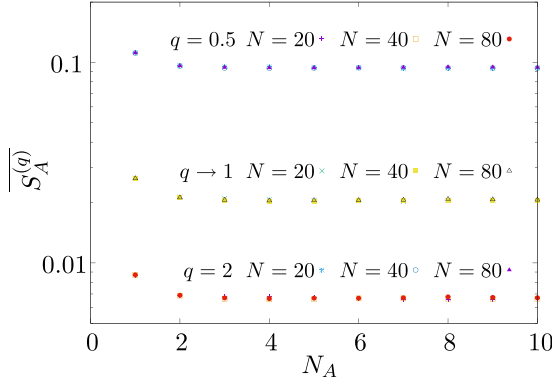
FIG. 1. Average entanglement entropy of METTS between the left part (sites $n \leqslant N_A$) and the right part (sites $n > N_A$) as a function of the size N_A of the subsystem A for the critical transverse-field Ising chain with $\nu = z$ and $\beta = 4$. Imaginary-time evolution is carried out using second-order Trotter decomposition with a time step $\delta\tau = 0.04$. The data are averaged over 10 000 samples.

central charge $c = 1/2$. Since this Hamiltonian does not have SU(2) spin rotation symmetry, the entanglement properties of METTS depend on the choice of the quantization axis ν. However, as will be seen later, the behavior of entanglement entropy at large β is independent of ν.

The second model is the spin-1/2 Heisenberg chain with the next-nearest-neighbor interaction,

$$H = \sum_{n=1}^{N-1} \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + S_n^z S_{n+1}^z \right)$$
$$+ J \sum_{n=1}^{N-2} \left(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y + S_n^z S_{n+2}^z \right). \quad (10)$$

Again, we take the open boundary condition. We set $J = 0.241\,167$ so that the model is critical [17–19]. This theory is well described by CFT with a central charge $c = 1$ [18]. This model is known to be not integrable [20].

As shown in Fig. 1, the entanglement profiles are insensitive to the length of the whole spin chain N or length

of the interval subsystem. Therefore, it is sufficient to consider the case where the interval A consists of the half chain $A = \{1, 2, \ldots, N/2\}$ for sufficiently large N to investigate the β dependence (see Supplemental Material [13] and also Refs. [14,21] therein). Then, in Fig. 2, we show the average entanglement Rényi entropy for the half chain as a function of β. For $\beta \gg 1$, we find

$$\overline{S_A^{(q)}} \simeq \frac{c}{12}\left(1 + \frac{1}{q}\right)\log\beta + S_0^{(q)}, \quad (11)$$

where $S_0^{(q)}$ is a nonuniversal constant. Furthermore, the standard deviation of the entanglement entropy of METTS is bounded by a constant and is negligible in the low-temperature limit as compared to the average. That is, at low temperatures, the entanglement Rényi entropy of METTS coincides with the entropy of the regularized boundary state (4) and a half of our upper bound by the entropy of the TFD state (8) at the leading order of β. This result is consistent with the intuition obtained from the discussion in the low-temperature limit pointed out in Ref. [8]. However, it is not immediately evident that the entanglement of METTS is half of the TFD state even in the finite-temperature region since the entanglement of the imaginary-time evolved state significantly depends on the choice of the initial state.

Computation time in the METTS algorithm. The area law and the logarithmically slow growth of the entanglement Rényi entropy (11) for $0 < q < 1$ implies that METTS can be efficiently represented by an MPS ansatz [4,5]. Hence it is expected that the METTS algorithm can be used to reach considerably low temperatures even for critical spin chains. With the results obtained above, let us evaluate the computation time in the METTS algorithm for simulating the canonical Gibbs state.

Consider a Schmidt decomposition of the METTS $|\mu_i\rangle = \sum_k \lambda_k |k\rangle_A |k\rangle_B$ with respect to the bipartition $A = \{1, 2, \ldots, N_A\}$ and its complement B. Suppose that the Schmidt coefficients λ_i's are sorted in decreasing order, i.e., $\lambda_1 \geqslant \lambda_2 \geqslant \cdots$. The truncation error for an MPS approximation of bond dimension D is defined as $\varepsilon \equiv \sum_{k>D} \lambda_k^2$. As shown in Ref. [4], ε measures an error in an MPS

(a) Ising model ($\nu = x$)　　　　　(b) Ising model ($\nu = z$)　　　　　(c) Heisenberg model
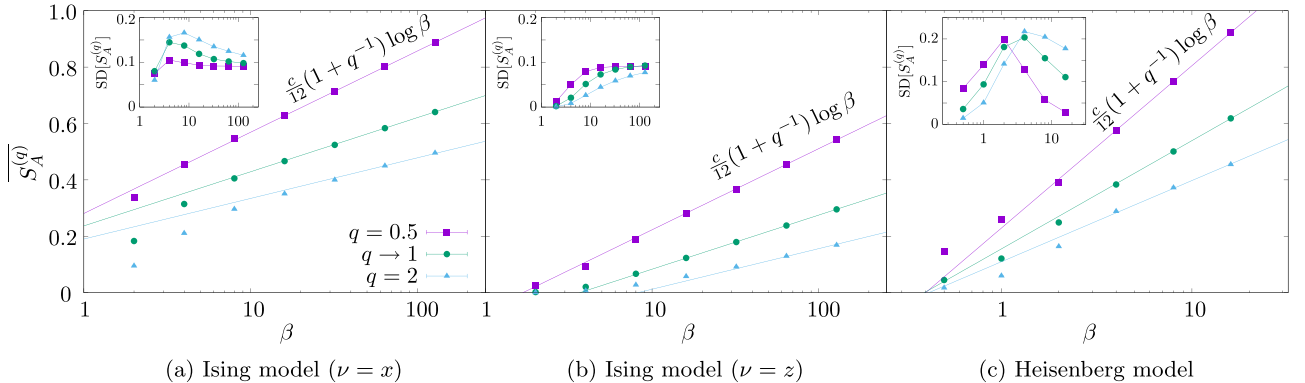
FIG. 2. Growth of the average entanglement Rényi entropy of METTS for the half chain $A = \{1, 2, \ldots, N/2\}$ (a), (b) in the critical transverse-field Ising model of length $N = 640$ and (c) in the critical Heisenberg model with the next-nearest-neighbor interaction of length $N = 1280$. The insets show the standard deviation of the entanglement Rényi entropy. Imaginary-time evolution is carried out using second-order Trotter decomposition with a time step $\delta\tau = 0.04$ for the Ising model and $\delta\tau = 0.01$ for the Heisenberg model. The data are averaged over 10 000 samples for the Ising model and 5000 samples for the Heisenberg model.
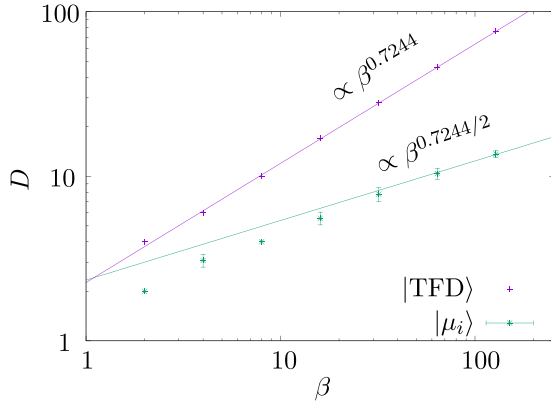
FIG. 3. Minimum bond dimension D necessary to approximate the TFD state and METTS with a truncation error of less than 10^{-10} for the critical transverse-field Ising chain with $N = 640$ sites. The data points for METTS are the average of D of 10 000 samples. The error bars indicate the standard deviation. We set the quantization axis ν to z. Imaginary-time evolution is carried out using second-order Trotter decomposition with a time step $\delta\tau = 0.04$.

approximation in the following sense: There exists an MPS $|\psi_D\rangle$ of bond dimension D such that $\| |\mu_i\rangle - |\psi_D\rangle \|_2^2 \leqslant 2 \sum_{N_A=1}^{N-1} \varepsilon$. Furthermore, ε can be bounded from above by

$$\log \varepsilon \leqslant \frac{1-q}{q}\left(S_A^{(q)} - \log \frac{D}{1-q}\right), \qquad (12)$$

for any $0 < q < 1$ [4]. By inverting this inequality, we find an upper bound on the bond dimension necessary to approximate the METTS within the truncation error ε:

$$\log D \leqslant S_A^{(q)} - \frac{q}{1-q}\log \varepsilon + \log(1-q). \qquad (13)$$

Substituting the numerical result (11), we get an upper bound on D for generic METTS scales as

$$\mathcal{O}\left(N^0 \beta^{\frac{c}{12}(1+q^{-1})}\right), \qquad (14)$$

for fixed ε and q. Note that the constant factor depends on ε and q, and hence it does not necessarily mean that the highest efficiency is achieved at $q = 1$. On the other hand, also for the TFD state, there is an upper bound on D that scales as [15]

$$\mathcal{O}\left(N^0 \beta^{\frac{c}{6}(1+q^{-1})}\right). \qquad (15)$$

Then we numerically check the bond dimension necessary to approximate the TFD state and METTS. In Fig. 3, we show the minimum bond dimension needed to achieve a truncation error ε of less than 10^{-10} for the TFD state and METTS as a function of β. We can confirm that the exponent on β for the TFD state is just twice that for generic METTS in the low-temperature limit. This is consistent with Eqs. (14) and (15).

According to Ref. [2], the computation time of the imaginary-time evolution for β scales as $ND^3\beta$. Therefore, we can efficiently produce METTS at sufficiently low temperatures with the computation time that scales as a polynomial in β with an exponent smaller than that of the TFD state.

We finally demonstrate the superiority of the METTS algorithm over the TFD algorithm at low temperatures by comparing the computation time in actual numerical
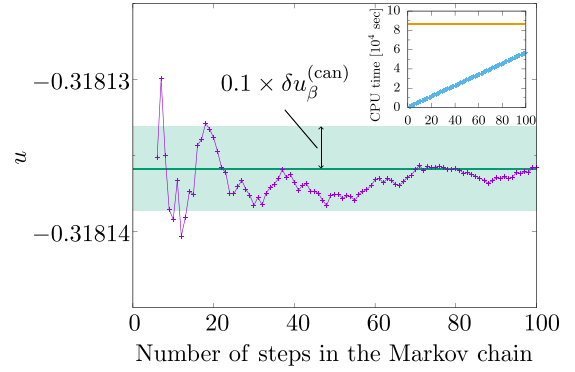

FIG. 4. Typical trajectory of the cumulative moving average of the energy per site $u = E/N$ in the Markov chain of the METTS simulation for the critical transverse-field Ising chain with $N = 640$ sites at $\beta = 128$. We set the quantization axis ν to z for the odd-numbered steps and x for the even-numbered steps to reduce correlations between successive samples [22]. To avoid initial transients, we discard the first five samples when calculating the sample averages. The solid line shows the result of the TFD approach, considered exact, and the shaded region shows a range of 0.1 times the standard deviation $\delta u_\beta^{(\text{can})}$ of u in $\rho_\beta^{(\text{can})}$ from the exact value. The inset shows the total computation time in the METTS simulation as a function of the number of steps in the Markov chain. The solid line shows the computation time in the TFD simulation.

simulations. To calculate expectation values in the canonical Gibbs state $\rho_\beta^{(\text{can})}$ via the METTS algorithm, we generate a Markov chain of METTS so that the long-time average coincides with $\rho_\beta^{(\text{can})}$ and then calculate the average of the expectation values in METTS sampled from that chain. Figure 4 depicts a typical trajectory of the cumulative moving average of the energy per site $u = E/N$ in METTS and the computation time in the METTS simulation. It can be seen that it only takes about 20 steps for sample averages to converge within a range of 0.1 times the standard deviation $\delta u_\beta^{(\text{can})}$ of u in $\rho_\beta^{(\text{can})}$ from the exact value. In other words, with only a few samples, we can correctly obtain the energy with an accuracy sufficiently smaller than the uncertainty inherent in the ensemble. Furthermore, we also observe that the total computation time for reaching that step is only about $1/8$ of that for the TFD algorithm. We therefore conclude that the METTS algorithm can provide a speedup over the TFD algorithm when analyzing low-temperature states in 1D gapless systems. However, in both algorithms, it is possible to reduce the computation time by increasing the Trotter error or truncation error within an allowable error range, and in such a case the TFD algorithm outperform the METTS algorithm [8]. Nevertheless, these errors are difficult to control, compared to statistical errors, which can be easily controlled by simply increasing the number of samples. In addition, in the case of the METTS algorithm, it is possible to parallelize the sampling to reduce the computation time.

Conclusions. In this Letter, we focus on evaluating the computational efficiency of the METTS algorithm for simulating low-temperature thermal equilibrium states in 1D gapless systems. We find it is efficient in the sense that the computation time scales as a polynomial function of β and has

a significant superiority compared to the TFD method. These are based on both the analytic upper bound and numerical investigations on the average entanglement Rényi entropy of METTS, which are motivated by a hint obtained in a BCFT computation.

We would like to emphasize that, although it was well known in the experience that a METTS usually requires fewer bond dimensions than a TFD state and the METTS algorithm takes less time than the TFD method in some cases, why and to what extent this is true was not well understood so far, both for gapped systems and gapless systems. More than justifying this experimental rule, our results also demonstrated that the speedup of METTS compared to TFD for simulating 1D gapless systems at low temperatures is parametrically large, i.e., the speedup gets larger as β gets larger, different from 1D gapped systems.

From a theoretical point of view, the average entanglement entropy of METTS is also capable of upper bounding the entanglement of formation for the canonical Gibbs state, which is defined as the minimum average entanglement over all of its possible pure state decompositions. This further bounds operational entanglement measures, such as distillable entanglement and entanglement cost. It is expected that the METTS decomposition is quite close to being optimal. Thus,

it is possible to obtain a tight bound on the entanglement of formation with the average entanglement of METTS. Therefore, by utilizing the results of this work, one can investigate the amount of entanglement in canonical Gibbs states.

Last but not least, METTS are low-entanglement atypical states mimicking thermal equilibrium. Translated to the language of quantum gravity via the anti–de Sitter (AdS)/CFT correspondence, this means METTS may be understood as black hole microstates which have nontrivial structures near the horizon [14]. Therefore, the statistical features of METTS may play an important role in understanding the microstate physics of black holes.

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[6] It is known that D for *general* METTS is upper bounded by $\mathcal{O}(e^{\sqrt{N\beta}})$ [23], which does not manifest the efficiency of METTS at low temperatures. However, we only need to upper bound the entanglement growth rate in *generic* METTS to evaluate the efficiency of the METTS algorithm. Therefore, there is large room for improvement.

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