Complexity of thermal states in quantum spin chains

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We study the quantum correlations and complexity of simulation, characterized by quantum mutual information and entanglement entropy in operator space, respectively, for thermal states in critical, noncritical, and quantum chaotic spin chains. A simple general relation between the two quantities is proposed. We show that in *all cases* mutual information and entanglement entropy saturate with system size, whereas as a function of the *inverse temperature*, we find *logarithmic divergences* for critical cases and uniform bounds in noncritical cases. A simple efficient quasiexact method for computation of arbitrary entropy-related quantities in thermalized *XY* spin chains is proposed.

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I. INTRODUCTION

The physical properties of nonintegrable strongly correlated quantum systems are notoriously difficult to calculate due to the exponential growth of the Hilbert-space dimension with system size. Nevertheless, many numerical and analytical approaches have been developed that provide results for special properties and specific systems. The question arises, which quantities are amenable to classical calculation in spite of generic system complexity?

Recently, two results emerging from the field of quantum information have shed light on the question. First, it has been shown that for one-dimensional (1D) systems the entanglement content of ground states grows logarithmically with the number of particles for fermionic critical systems and saturates for noncritical or bosonic systems [1–4]. Second, the *density matrix renormalization group* (DMRG) method [5] has been reinterpreted and optimized within *the matrix product state* (MPS) ansatz [6,7] for the many-body wave function. Its complexity is essentially given by the *entanglement entropy* of the system's bipartition. Despite being essentially the best method available, it is not known precisely in which instances is the DMRG method computationally efficient; for example, it has been shown to be *inefficient* for computing the evolution of *homogeneous* 1D nonintegrable systems in *real* time [8], but becomes efficient in the presence of *disorder* due to the emergence of (many-body) localization [9]. Thermal states at finite temperature have been simulated using an extension of the MPS ansatz to density operators [*matrix product operators* (MPOs)] and by performing the evolution in *imaginary time* (inverse temperature) [7]. However, no analysis of efficiency scaling with the system size n and inverse temperature β has been performed. Note that finding a ground state—corresponding to the limit $\beta\to\infty$—is proven to be a difficult problem [10], even though it can often be performed efficiently [5]. For a different algorithm for computing thermal states see Ref. [11]. In Ref. [12] an upper bound on the necessary MPO dimension is found for thermal states which unfortunately scales exponentially with β. It is not clear if one can do better—that is, if finite-temperature states can be calculated efficiently, uniformly in β. In the present work we show that this is indeed possible.

Complexity will be characterized by the *operator-space entanglement entropy* (OSEE) [13] of thermal states which is directly linked to the minimal necessary rank of the MPO ansatz. OSEE is defined as von Neumann entropy of the reduced density matrix defined with respect to a physical density operator treated as an element of a Hilbert (Fock) space of operators. In addition we shall show that OSEE behaves in the same way as the *quantum mutual information* (QMI) $I_{A:B}$ [14], which is a natural measure of quantum correlations in a bipartition $A+B$ and an *upper bound* for distillable entanglement. Our main result is that OSEE and $I_{A:B}$ in the thermodynamic limit $n\to\infty$ grow as $\sim(c/3)\log_2\beta$ for critical (gapless) systems and *saturate* for noncritical (gapped) systems, while they *always saturate* with β for a finite n. This shows that the linear in β upper bound on QMI of Ref. [15] is far from optimal and DMRG computations of large (infinite) critical 1D quantum systems should be *efficient* at *all nonzero* temperatures. This has to be contrasted with typical *linear* growth of OSEE in t in *real time* evolution [8]. Note that OSEE and QMI always saturate with n, for any fixed β, and hence scale very differently from thermodynamic entropy of a block of length n, which for a critical system behaves as [16] $S\propto\frac{n}{\beta}$ for large n. Our results are based on analytical and numerical calculations in several examples of integrable and nonintegrable spin chains. We outline a method for quasiexact calculations of OSEE and $I_{A:B}$ in *XY* spin-1/2 chains using the concept of Fock space of operators [17], whereas we rely on numerical MPO-DMRG simulations for the other cases.

II. METHODS

First, we describe how to construct a thermal state and compute OSEE in a general spin chain, regardless of its integrability, using the MPO ansatz and imaginary-time evolution. A thermal state $\rho(\beta)=\exp(-\beta H)/\mathrm{tr}[\exp(-\beta H)]$ of Hamiltonian H of a chain of n spins 1/2 can be expressed as an element of 4^n-dimensional Hilbert space $\mathcal{K}$, $|\rho\rangle=\Sigma_{\underline{s}}c_{\underline{s}}|\sigma^{\underline{s}}\rangle$, spanned by Pauli operators $\sigma^{\underline{s}}\equiv\sigma_1^{s_1}\cdots\sigma_n^{s_n}$, $\underline{s}\equiv s_1,\ldots,s_n$, $s_m\in\{0,1,2,3\}$, $\sigma^0\equiv\mathbb{1}$, $\sigma^{1,2,3}\equiv\sigma^{x,y,z}$. The inner product in $\mathcal{K}$ is defined as $\langle x|y\rangle=2^{-n}\mathrm{tr}x^\dagger y$. Within the MPO ansatz expansion coefficients $c_{\underline{s}}$ are represented in terms of $4n$ $D\times D$ matrices $\mathbf{A}_m^s$, $m=1,\ldots,n$, $s=0,1,2,3$, as

$$c_{\underline{s}} = \mathrm{tr}(\mathbf{A}_1^{s_1} \cdots \mathbf{A}_n^{s_n}). \quad (1)$$

For the exact MPO representation the matrix dimension of $\mathbf{A}_m^s$ must be equal to the number of nonzero Schmidt coefficients for a bipartite cut of a vector $c_{\underline{s}}$ at the corresponding site. Although for generic density operators ρ the required dimension D is exponentially large (in n), in practice one truncates the matrices to a smaller dimension D and uses (1) as a variational ansatz. As a rough estimate of a minimal $D \sim 2^{S^\sharp}$, which is a direct measure of *complexity* of ρ, one can use OSEE $S^\sharp$ defined as an *entanglement entropy* of a superket $|\rho\rangle$:

$$S^\sharp = -\mathrm{tr}_A(\mathbf{R}\log_2 \mathbf{R}), \quad \mathbf{R} = \langle\rho|\rho\rangle^{-1}\,\mathrm{tr}_B|\rho\rangle\langle\rho|, \quad (2)$$

where a subscript A denotes the first n_A sites and B its complement. A more detailed analysis [18] specifies exact criteria for the applicability of the matrix product ansatz (1) in terms of properties of the moments of Schmidt coefficients. Writing the expansion coefficients $c_{\underline{s}}$ as a $(2^{n_A}\times 2^{n-n_A})$-dimensional matrix $C_{\underline{s}_A,\underline{s}_B}=c_{\underline{s}_A\underline{s}_B}$, the reduced density matrix (2) is given by $\mathbf{R}=\mathbf{C}\mathbf{C}^T/\mathrm{tr}(\mathbf{C}\mathbf{C}^T)$ and quantifies the bipartite correlations and the difficulty of a MPO simulation of a given density operator ρ. For the use of OSEE in a non-MPO context, see Ref. [19]. $S^\sharp$ is directly related to the entanglement entropy of physical states only in the case of pure states, $\rho=|\psi\rangle\langle\psi|$, in which case $S^\sharp$ is just twice the entanglement entropy of a pure state ψ—e.g., the ground state at zero temperature. However, even though $S^\sharp$ is not an entanglement monotone for general ρ, it can be used as a bipartite entanglement estimator for thermal states $\rho(\beta)$. Namely, as we will demonstrate later, its scaling on n and β is the same as that of QMI $I_{A:B}$, defined as

$$I_{A:B} = S(\rho_A) + S(\rho_B) - S(\rho), \quad (3)$$

where $\rho_A=\mathrm{tr}_B\rho$, $\rho_B=\mathrm{tr}_A\rho$, and $S(\sigma)=-\mathrm{tr}(\sigma\log_2\sigma)$. QMI measures total correlations between A and B and is an upper bound for relative entropy of entanglement, which in turn is an upper bound for distillable entanglement $E_D(\rho)$ [20]. The MPO representation for a thermal state $\rho(\beta)$, apart from normalization, is computed by performing imaginary-time evolution in β, $\rho(\beta+\epsilon)=\exp(-\epsilon H/2)\rho(\beta)\exp(-\epsilon H/2)$, starting at an infinite-temperature state $\rho(0)=\mathbb{1}/2^n$ having $D=1$. Such β evolution increases OSEE and, as a consequence, dimension D has to increase as well in order to preserve the accuracy. Assuming the empirical fact that a *fixed* small ϵ (in our case $\epsilon=0.05$) is enough to produce accurate results in a *finite* number of steps (for all $\beta<\infty$), we conclude that the time complexity of simulation is polynomial in D and β. Note that in contrast to a (unitary) *real-time* evolution, imaginary-time evolution does not preserve canonical Schmidt decomposition structure of matrices $\mathbf{A}_m^{s_m}$ [6]. In order to improve stability we apply local rotations every few steps in order to "reorthogonalize" the matrices $\mathbf{A}_m^{s_m}$.

Quasiexact calculation of $S^\sharp$ and $I_{A:B}$ for thermal states is possible for integrable chains which can be mapped to quadratic fermionic models by Wigner-Jordan transformation—e.g., the 1D XY model. The most general such situation is described by a Hamiltonian $H=\underline{w}\cdot\mathbf{H}\underline{w}\equiv\sum_{j,l=1}^{2n}H_{jl}w_jw_l$, where $\mathbf{H}$ is an *antisymmetric Hermitian* $2n\times 2n$ matrix and $w_{2m-1}=\sigma_m^x\prod_{l=1}^{m-1}\sigma_l^z$, $w_{2m}=\sigma_m^y\prod_{l=1}^{m-1}\sigma_l^z$ are Majorana operators satisfying $\{w_j,w_l\}\equiv w_jw_l+w_lw_j=2\delta_{jl}$. It is crucial to recognize [13,17] that $\mathcal{K}$ is in fact a *Fock space* if spanned by 4^n products of w_j, $P_{\underline{\alpha}}=w_1^{\alpha_1}\cdots w_{2n}^{\alpha_{2n}}$, $\alpha_j\in\{0,1\}$, and equipped with adjoint Fermi maps $\hat{c}_j|P_{\underline{\alpha}}\rangle=\delta_{\alpha_j,1}|w_jP_{\underline{\alpha}}\rangle$. In our notation the caret designates a linear map over the Fock space of operators $\mathcal{K}$. Note that OSEE is just an entanglement entropy of an element of $\mathcal{K}$. Therefore, using the formalism of [2] lifted to an operator space, one can calculate $S^\sharp$ from the *antisymmetric* correlation matrix $\mathbf{\Gamma}$ defined by

$$\frac{\langle e^{-\beta H}|\hat{a}_p\hat{a}_q|e^{-\beta H}\rangle}{\langle e^{-\beta H}|e^{-\beta H}\rangle} = \delta_{pq} + i\Gamma_{pq}, \quad p,q=1,\ldots,4n, \quad (4)$$

where $\hat{a}_{2j-1}\equiv(\hat{c}_j+\hat{c}_j^\dagger)$ and $\hat{a}_{2j}\equiv i(\hat{c}_j-\hat{c}_j^\dagger)$, $j=1,\ldots,2n$, satisfying $\{\hat{a}_p,\hat{a}_q\}=2\delta_{pq}$. The thermal state in (4) can be written in terms of dynamics,

$$|e^{-\beta H}\rangle = \exp(-\beta\hat{\mathcal{H}})|\mathbb{1}\rangle, \quad (5)$$

using a quadratic adjoint Hamiltonian map $\hat{\mathcal{H}}$ over $\mathcal{K}$, $\hat{\mathcal{H}}=(\hat{\underline{c}}+\hat{\underline{c}}^\dagger)\cdot\mathbf{H}(\hat{\underline{c}}+\hat{\underline{c}}^\dagger)$, since $(\hat{c}_j+\hat{c}_j^\dagger)|\rho\rangle=|w_j\rho\rangle$. Diagonalizing the matrix $\mathbf{H}$ we obtain eigenvalues $\lambda_k,-\lambda_k$, ordered such that $0\leqslant\lambda_1\leqslant\cdots\leqslant\lambda_n$, and the corresponding *orthonormal* eigenvectors $\underline{v}_k$ and $\underline{v}_k^*$, in terms of which we write the adjoint Hamiltonian in (5) in the *normal form* $\hat{\mathcal{H}}=\sum_{k=1}^n 4\lambda_k(\hat{b}_k^\dagger\hat{b}_k-\frac{1}{2})$, where $\hat{b}_k=\underline{v}_k^*\cdot(\hat{\underline{c}}+\hat{\underline{c}}^\dagger)/\sqrt{2}$. Identities $\langle\mathbb{1}|\hat{b}_k|\mathbb{1}\rangle=0$, $\langle\mathbb{1}|\hat{b}_k\hat{b}_l|\mathbb{1}\rangle=0$ and $\langle\mathbb{1}|\hat{b}_k^\dagger\hat{b}_l|\mathbb{1}\rangle=\frac{1}{2}\delta_{kl}$ allow us to employ the Wick theorem to evaluate (4):

$$\Gamma_{2j-1,2l-1} = -\Gamma_{2j,2l} = -2\sum_{k=1}^n \tanh(4\beta\lambda_k)\mathrm{Im}(v_{k,j}^*v_{k,l}),$$

$$\Gamma_{2j,2l-1} = \delta_{jl} - 2\sum_{k=1}^n\left(1-\frac{1}{\cosh(4\beta\lambda_k)}\right)\mathrm{Re}(v_{k,j}^*v_{k,l}). \quad (6)$$

Finally, OSEE is obtained from the eigenvalues $\pm i\nu_j$ of the $4n_A\times 4n_A$ upper-left block of $\mathbf{\Gamma}$ as $S^\sharp=\sum_{j=1}^{2n_A}H_2(\frac{1+\nu_j}{2})$ where $H_2(x)=-x\log_2 x-(1-x)\log_2(1-x)$ [2].

Similarly, we can also easily compute the block entropy $S(\rho_A)$ of a thermal state $\rho(\beta)$ by diagonalizing $H=\sum_{k=1}^n 4\lambda_k(b_k^\dagger b_k-\frac{1}{2})$, with operators $b_k=\underline{v}_k^*\cdot\underline{w}/\sqrt{2}$ (which are elements of $\mathcal{K}$ and not maps over $\mathcal{K}$ like $\hat{b}_k$) and computing the correlation matrix $\mathbf{\Gamma}'$, defined as $\mathrm{tr}(w_jw_le^{-\beta H})/\mathrm{tr}e^{-\beta H}=\delta_{jl}+i\Gamma'_{jl}$, $j,l=1,\ldots,2n$. Expressing w_j and H in terms of b_k and $b_k^\dagger$ and using the Wick theorem with $\mathrm{tr}(b_k^\dagger b_l)=\frac{1}{2}\delta_{kl}\mathrm{tr}\mathbb{1}$ results in a general two-point thermal correlation function

$$\Gamma'_{jl} = -2\sum_{k=1}^n \tanh(2\beta\lambda_k)\mathrm{Im}(v_{k,j}^*v_{k,l}). \quad (7)$$

Diagonalizing the $2n_A\times 2n_A$ block of Γ' corresponding to the sublattice A, yielding eigenvalues $\pm i\nu'_j$, we obtain the block entropy $S(\rho_A)=\sum_{j=1}^{n_A}H_2(\frac{1+\nu'_j}{2})$. Considering also B, and $A+B$ instead of A, we get QMI (3).

III. RESULTS

We shall show results for OSEE and QMI for several families of critical and noncritical as well as integrable and nonintegrable quantum spin chains:

$$H_{XY} = \sum_{l=1}^{n-1} \left(\frac{1+\gamma}{2} \sigma_l^x \sigma_{l+1}^x + \frac{1-\gamma}{2} \sigma_l^y \sigma_{l+1}^y \right) + \sum_{l=1}^{n} h \sigma_l^z,$$

$$H_I = \sum_{l=1}^{n-1} \sigma_l^x \sigma_{l+1}^x + \sum_{l=1}^{n} (h_x \sigma_l^x + h_z \sigma_l^z),$$

$$H_{XXZ} = \sum_{l=1}^{n-1} (\sigma_l^x \sigma_{l+1}^x + \sigma_l^y \sigma_{l+1}^y + \Delta \sigma_l^z \sigma_{l+1}^z) + \sum_{l=1}^{n} h_l \sigma_l^z, \quad (8)$$

all for open boundary conditions, and a symmetric cut at $n_A = n/2$, where largest bipartite entanglement is expected. The Majorana representation of the integrable XY case which is necessary for explicit calculations [Eqs. (4)–(7)] is $H_{XY} = -i\Sigma_{l=1}^{n-1}(\frac{1+\gamma}{2} w_{2l} w_{2l+1} - \frac{1-\gamma}{2} w_{2l-1} w_{2l+2}) - i\Sigma_{l=1}^{n} h w_{2l-1} w_{2l}$.

In Fig. 1 we show the results for *quantum critical* systems for which the entanglement entropy of the ground state grows as $S_0 \sim (c/3)\log_2 n$ [2], where c is the central charge of the corresponding conformal field theory [3]. However, we take several very large n and plot β dependence of OSEE and QMI, for the (a) XX model $H_{XY}(\gamma=0, h=0)$, (b) transverse Ising model $H_{XY}(\gamma=1, h=1)$, and (c) XXZ model $H_{XXZ}(\Delta=0.5, h_l \equiv 0)$. These critical models are all completely integrable; however, we were able to make exact calculations only for (a) and (b), whereas we used MPO-DMRG simulations for (c) where—since evaluating QMI (3) is computationally difficult even within the MPO ansatz—we have instead computed *mutual purity*, defined as $I_P = \log_2\{P(\rho)/[P(\rho_A)P(\rho_B)]\}$ with $P(\sigma) = \mathrm{tr}\sigma^2$. It is well known that purity often well describes the behavior of von Neumann entropy and its complement is sometimes termed linear entropy. In addition we checked for thermal states of small systems that mutual purity and QMI behave similarly.

From Fig. 1 we conclude that in the large-n limit OSEE grows logarithmically with β:

$$S^{\#}(\beta) = \frac{c}{3} \log_2 \beta + c', \quad (9)$$

with parameters $c=1$ and $c'=1.17$ for the XX model (a), $c=1/2$ and $c'=0.75$ for transverse Ising model (b), and $c=1$ and $c'=1.63$ for XXZ model (c). c is exactly the central charge of the corresponding model. Presently we do not have an explanation for this finding and we state it as a conjecture. For fixed n, $S^{\#}$ saturates for β larger than the inverse spectral gap $\beta^* = 1/\Delta E$ at twice the ground-state value, $2S_0 \sim (2c/3)\log_2 n$.

Next, let us have a look at *noncritical* systems. First, we will chose two *nonintegrable* spin models that display typical signatures of quantum chaos (Fig. 2): (a) the Heisenberg XXZ model in a *staggered* magnetic field H_{XXZ} ($\Delta=0.5$, $h_l = -[1+(-1)^l]/2$) and (b) Ising model in a tilted magnetic field $H_I(h_x=1, h_z=1)$. We can see that for non critical systems which possess a finite energy gap ΔE between the ground and first excited states, OSEE *saturates* at n and β independent values for sufficiently large $\beta \gg \beta^*$, so the classical simulation of quantum thermal states for gapped systems is even more efficient than for critical ones. Although this might seem expected, one should know that for OSEE we do not have theoretical uniform bounds in n like for QMI [15]. Note that in the presence of weakly broken symmetries, the gap ΔE between two lowest states can become exponentially small with n even though the system is not critical. This for instance happens in the XY model. In Fig. 3 we show results for a noncritical integrable XY model (8) with $\gamma=0.5$ and $h=0.9$, where $\beta^* = 1/\Delta E$ grows exponentially with n. Actually we have shown for any H_{XY} that $\Delta E = 4\lambda_1$, where λ_1 is the smallest eigenvalue of matrix $\mathbf{H}$, Eq. (5), and which in turn has been found to decay exponentially, $\lambda_1 \sim \exp(-n/\xi)$. Interestingly, for $h^2+\gamma^2<1$, the decay length ξ is practically *insensitive* to parameters γ and h, whereas at the point $h^* = \sqrt{1-\gamma^2}$, where the ground state is doubly degenerate and separable [21], ξ instantly starts increasing with increasing $h-h^*$ (inset of Fig. 3). However, there is no phase transition at h^*.

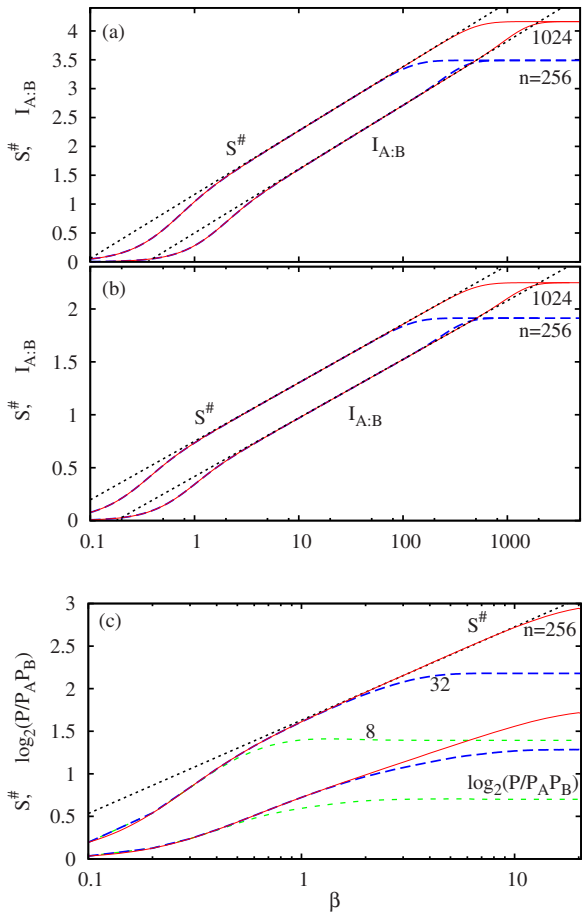

FIG. 1. (Color online) Logarithmic growth of OSEE $S^{\#}$ (upper curves) and QMI $I_{A:B}$ (lower curves) for thermal states of critical models: (a) XX chain $H_{XY}(\gamma=0, h=0)$, (b) transverse Ising chain $H_{XY}(\gamma=1, h=1)$, both for $n=1024, 256$, and (c) XXZ chain $H_{XXZ}(\Delta=0.5, h_l \equiv 0)$ for $n=256, 32, 8$. In case (c) we show mutual purity I_P instead of $I_{A:B}$. Dotted lines indicate conjectures (9) and (10) combined with (9) (see text).

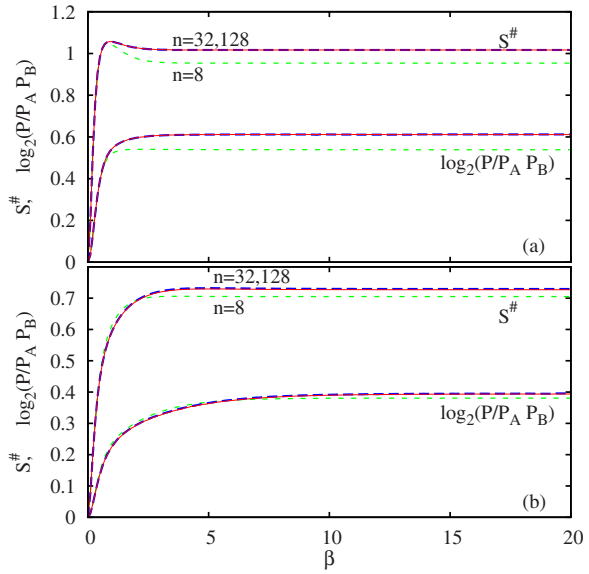

FIG. 2. (Color online) Saturation of OSEE $S^\sharp$ (upper curves) and mutual purity I_P (lower curves) for quantum chaotic *noncritical* systems—namely, (a) for the *XXZ* model in a staggered field $H_{XXZ}(\Delta=0.5, h_l=-[1+(-1)^l]/2)$ and (b) for tilted Ising $H_I(h_x=1, h_z=1)$, for $n=8, 32, 128$. Note that the curves for $n=32$ and $n=128$ are practically indistinguishable.

In all cases studied QMI behaves in essentially the same way as OSEE. In fact, for models solvable by Wigner-Jordan transformation $I_{A:B}(\beta)$ almost overlaps with $S^\sharp$ evaluated at $\beta/4$,

$$I_{A:B}(\beta) \approx S^\sharp(\beta/4), \tag{10}$$

apart from finite-size effects at small and large β (Figs. 1 and 3). We conjecture that (10) becomes asymptotically exact for large n. The factor of 4 may be understood from comparing the formalisms of Majorana operators w_j and the adjoint maps $\hat{c}_j$. Since QMI is an upper bound for distillable entanglement [20], this means that exact quantum bipartite entanglement for thermal states is also small; i.e., it is either upper bounded by n- and β-independent values for noncritical systems (Figs. 2 and 3) or it is upper bounded by the n-independent value $\sim \log_2 \beta$ for critical systems.

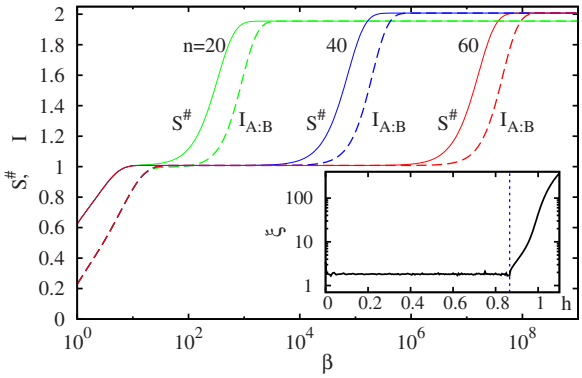

FIG. 3. (Color online) OSEE $S^\sharp$ (solid curves) and QMI $I_{A:B}$ (dashed curves) for a *noncritical XY* chain with $\gamma=0.5$, $h=0.9$, and $n=20, 40, 60$. Note a crossover between two saturation plateaus due to a single exponentially close (in n) excited state. The inset shows the h dependence of the gap decay length ξ, computed from the fit to $\Delta E \propto e^{-n/\xi}$, for $n=30, \ldots, 60$. The vertical line indicates $h^* = \sqrt{1-\gamma^2}$.

IV. CONCLUSIONS

By studying several typical models, we have demonstrated that classical simulations of thermal states of interacting quantum systems in 1D are *efficient*. Using DMRG simulations combined with exact calculations for *XY* models we found that in noncritical systems complexity and bipartite entanglement measures are uniformly bounded, in both system size n and inverse temperature β, whereas they exhibit a universal logarithmic divergence in inverse temperature for quantum critical systems.

Our results represent a *uniform* finite-temperature extension of the ground-state *area law* [1,2,15]. Specifically, for critical systems, the logarithmic divergence of the ground-state block entropy with the size of the block is reflected in the logarithmic divergence in the inverse temperature β of the bipartite entanglement of thermal (mixed) states in the thermodynamic limit. Even though our results are not rigorous, they suggest optimal bounds on entanglement and complexity of thermal states that are qualitatively stronger than previously known [15].

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