Entropy, Entanglement, and Area: Analytical Results for Harmonic Lattice Systems

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We revisit the question of the relation between entanglement, entropy, and area for harmonic lattice Hamiltonians corresponding to discrete versions of real free Klein-Gordon fields. For the ground state of the d-dimensional cubic harmonic lattice we establish a strict relationship between the surface area of a distinguished hypercube and the degree of entanglement between the hypercube and the rest of the lattice analytically, without resorting to numerical means. We outline extensions of these results to longer ranged interactions, finite temperatures, and for classical correlations in classical harmonic lattice systems. These findings further suggest that the tools of quantum information science may help in establishing results in quantum field theory that were previously less accessible.

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Imagine a distinguished geometrical region of a discretized free quantum Klein-Gordon field: What is the entropy associated with a pure state obtained by tracing over the field variables outside the region? How does this entropy relate to properties of the region, such as volume and boundary area? These innocent-looking questions pose a long-standing issue indeed, studied in the literature under the key word of "geometric entropy." Analytical steps supplemented by numerical computations for half spaces and spherical configurations in the seminal works by Bombelli *et al.* [1] and Srednicki [2] strongly suggested a direct connection between entropy and area. The interest in this quantity for quantum field theory was originally drawn from the fact that geometric entropy is a candidate for the Bekenstein-Hawking black hole entropy [3]. Subsequent work employed various approaches, such as methods from conformal field theory [4], analysis of entropy subadditivity [5], or mode counting [6]. While the connection to the black hole entropy and other concepts such as the holographic bound has not been fully clarified yet [7], the connection between entanglement and area in nongravitating systems is interesting in itself. Recently, there has been renewed interest in studying entanglement and correlations in quantum many-body systems and quantum field theory, largely due to the availability of novel powerful methods from the quantitative theory of entanglement in the context of quantum information theory [8–14]. Such ideas have previously been employed to assess the entanglement in settings of one-dimensional spin (see, e.g., Refs. [13,14]) and harmonic chains [10,12].

The analysis in this Letter is based on methods that have been developed in recent years in quantum information theory, in particular, those relating to entanglement in Gaussian (quasifree) states (see, e.g., Ref. [15]). These methods allow us to give an analytical answer to the question of the scaling of the degree of entanglement between a region and its exterior for harmonic lattice Hamiltonians such as discrete versions of the free scalar Klein-Gordon field, in arbitrary spatial dimensions. It is remarkable that although we encounter a highly correlated system, we nevertheless find an "area dependence" of the degree of entanglement.

The Hamiltonian.—The starting point of the argument is a discrete lattice version of a free real scalar quantum field. For any $d \geq 1$ we consider a d-dimensional simple cubic lattice $n^{\times d}$ comprising n^d oscillators. Denoting the canonical coordinates of the system by $\mathbf{x} = (x_1, \ldots, x_{n^d})$ and $\mathbf{p} = (p_1, \ldots, p_{n^d})$ we may write the Hamiltonian as

$$H = \mathbf{p}\mathbf{p}^{\mathrm{T}}/2 + \mathbf{x}V\mathbf{x}^{\mathrm{T}}/2. \tag{1}$$

The $n^d \times n^d$ matrix V, the potential matrix, specifies the coupling between the oscillators in the position coordinates. For now we chose V such that in the continuum limit one obtains the Hamiltonian of the real Klein-Gordon field. We therefore consider the harmonic lattice Hamiltonian with nearest-neighbor interaction. The case of next-to-nearest-neighbor coupling is discussed later in this Letter. For a discussion of more general types of interactions, see Ref. [16].

We write $V = \mathrm{circ}(\mathbf{v})$ for the circulant matrix whose first row is given by the n-tupel $\mathbf{v}$, and also for a block-circulant matrix where the first block column is specified by a tupel of matrices. So in $d = 1$ we have $V_1 = \mathrm{circ}(1, -c, 0, \ldots, 0, -c)$, and in higher dimensions we have, with $0 \leq c < 1/(2d)$, a recursive, block-circulant structure reflecting rows, layers, etc., $V_d = \mathrm{circ}(V_{d-1}, -c\mathbb{1}_{n^{d-1}}, 0, \ldots, 0, -c\mathbb{1}_{n^{d-1}})$. From now on we write V instead of V_d.

Entanglement and area dependence.—We denote the ground state of the system by ρ. For a distinguished cubic region $m^{\times d}$ in a lattice $n^{\times d}$ (see Fig. 1) its entropy of entanglement is $E_{n,m} = -\mathrm{tr}\, \rho_{n,m} \log \rho_{n,m}$. The reduced density matrix $\rho_{n,m}$ is formed by tracing out the variables outside the region $m^{\times d}$. We show that

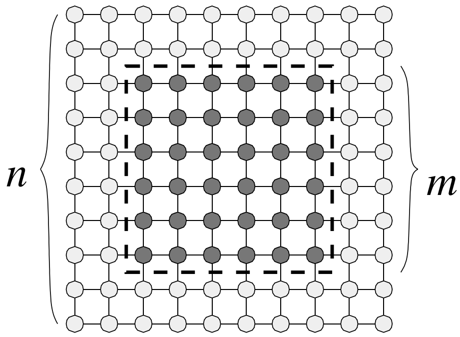

FIG. 1. The harmonic lattice in $d = 2$ with a distinguished $m \times m$ region in an $n \times n$ lattice.

The entropy of entanglement of the distinguished region $m^{\times d}$ in the lattice $n^{\times d}$ satisfies $\lim_{n\to\infty} E_{n,m} = \Theta(m^{d-1})$, where Θ is the Landau theta. More specifically, we have that $C_1 m^{d-1} \leq E_{n,m} \leq C_2 m^{d-1}$ for sufficiently large m, with appropriate $C_1, C_2 > 0$.

The area dependence manifests itself as follows: For a linear chain, the entropy of entanglement is bounded by quantities that are independent of the size of the distinguished interval. In two dimensions, this dependence is linear in the length of the boundary, and in three dimensions to the area of the boundary. Indeed, one can show that while all oscillators are correlated with all oscillators, the correlations over the boundary decay very quickly. In effect, for fixed interaction strength [17], the only significant contribution comes from within a finite width, the correlation length, along the boundary, and thus leads to a surface dependence of the correlations. This intuition forms the basis of the following, fully analytical proof.

The upper bound.—The ground state ρ of the coupled harmonic system in Eq. (1) is a Gaussian (quasifree) state with vanishing first moments. The second moments of ρ can be collected in the covariance matrix γ, which is defined as $\gamma_{j,k} = 2\,\mathrm{Re}[R_j R_k \rho]$ for $j, k = 1, \ldots, 2n^d$, where $\mathbf{R} = (\mathbf{x}, \mathbf{p})$ is the vector of canonical coordinates. In terms of the potential matrix V the covariance matrix of the ground state is then found to be $\gamma = V^{-1/2} \oplus V^{1/2}$ [10]. From entanglement theory we know that an upper bound for the entropy of entanglement is provided by the logarithmic negativity $E_N = \ln\|\rho^\Gamma\|_{\mathrm{tr}}$, where ρ^Γ is the partial transpose of ρ, and $\|\cdot\|_{\mathrm{tr}}$ denotes the trace norm [18]. Following Ref. [10] we find

$$E_N = \sum_{j=1}^{n^d} \ln\{1 + \max[0, \lambda_j(Q - \mathbb{1})]\}, \tag{2}$$

where $\lambda_j(Q)$ are the nonincreasingly ordered eigenvalues of the matrix

$$Q = V^{-1/2} P V^{1/2} P. \tag{3}$$

In a reordered list of canonical coordinates (such that the inner oscillators are counted first) P is the diagonal matrix $P = -\mathbb{1}_{m^d} \oplus \mathbb{1}_{n^d - m^d}$ and we define

$$V^{-1/2} = \begin{bmatrix} A & B \\ B^{\mathrm{T}} & C \end{bmatrix}, \quad V^{1/2} = \begin{bmatrix} D & E \\ E^{\mathrm{T}} & F \end{bmatrix}, \quad T = \begin{bmatrix} 0 & E \\ E^{\mathrm{T}} & 0 \end{bmatrix}.$$

The matrices B and E describe the couplings between the m^d oscillators forming the distinguished hypercube and the rest of the lattice. Using $V^{-1/2} V^{1/2} = \mathbb{1}$, we arrive at

$$Q - \mathbb{1} = -2V^{-1/2} T.$$

We replace the maximum in Eq. (2) by an absolute value and use that $\ln(1 + x) \leq x$ for all $x \geq 0$ so that $E_N \leq \sum_{j=1}^{n^d} \ln[1 + |\lambda_j(Q - \mathbb{1})|] \leq \|Q - \mathbb{1}\|_{\mathrm{tr}}$. Using the unitary invariance of the trace norm [19] and the fact that $V^{-1/2}$ is symmetric we obtain

$$\|Q - \mathbb{1}\|_{\mathrm{tr}} = 2\|V^{-1/2} T\|_{\mathrm{tr}} \leq 2\lambda_1(V^{-1/2}) \|T\|_{\mathrm{tr}}.$$

The spectrum of V can be obtained via discrete Fourier transform and yields $\lambda_1(V^{-1/2}) = (1 - 2cd)^{-1/2}$.

Now $\|T\|_{\mathrm{tr}}$ can be bounded from above by the sum of the absolute values of all the matrix elements of T, which is known as the l_1 matrix norm [19]. Therefore, $E_N \leq 2(1 - 2cd)^{-1/2} \sum_{i,j=1}^{n^d} |T_{ij}|$. In the following we bound the matrix elements of $V^{1/2}$ and consequently those of T. The explicit implementation of the multidimensional discrete Fourier transform is nontechnical yet involved. A more compact notation employs the coordinate vectors $\mathbf{k}, \mathbf{l}$ where $k_j, l_j = 0, \ldots, n - 1$ and $j = 0, \ldots, d - 1$. For our lattice we may write $V_{\mathbf{k},\mathbf{l}} = V_{\sum_{j=0}^{d-1} k_j n^j, \sum_{j=0}^{d-1} l_j n^j}$ for the interaction term between site $\mathbf{k}$ and $\mathbf{l}$. The matrix elements of $V^{1/2}$ are then given by

$$V^{1/2}_{\mathbf{k},\mathbf{l}} = \sum_{\mathbf{k}'} \prod_{j=0}^{d-1} \frac{e^{2\pi i k'_j (k_j - l_j)/n}}{n^d} \left(1 - 2c \sum_{r=0}^{d-1} \cos\frac{2\pi k'_r}{n}\right)^{1/2}.$$

To bound these, we replace the square root by its power series expansion in the parameter $2c$. This converges if $2cd \leq 1$, which coincides with the constraint imposed by the positivity of the potential matrix. We use $(1 - x)^{1/2} = 1 - \sum_{s=1}^{\infty} B_s x^s$, with $0 < B_s < 1$ and the fact that $\sum_{q=1}^{n} e^{2\pi i p q/n} = 0$ for integer p and q unless p is a multiple of n. Then, for $\mathbf{k} \neq \mathbf{l}$ we find

$$y^{s(\mathbf{k},\mathbf{l})}/(1 - y) \geq V^{-1/2}_{\mathbf{k},\mathbf{l}} \geq 0 \geq V^{1/2}_{\mathbf{k},\mathbf{l}} \geq -y^{s(\mathbf{k},\mathbf{l})}/(1 - y),$$

where $s(\mathbf{k}, \mathbf{l}) = (k_0 - l_0) + \cdots + (k_{n-1} - l_{n-1})$, $y = 2cd$, and $0 \leq k_j - l_j \leq n/2$. The remaining matrix elements are determined by the periodic boundary conditions under the exchange $k_j - l_j \mapsto n - (k_j - l_j)$. Note that $s(\mathbf{k}, \mathbf{l})$ is the *minimal* number of lattice steps to move from site $\mathbf{k}$ to site $\mathbf{l}$. If, for example, $s(\mathbf{k}, \mathbf{l}) = 1$, then the oscillators are direct neighbors.

We may now proceed with the computation of the l_1 norm of T, i.e., of the blocks in $V^{1/2}$ that describe the coupling between the distinguished region and the rest of the lattice. Given that the region is a hypercube, this can be done in a transparent way. Consider the set $\mathcal{L}_0$ of $m^d - (m-2)^d$ oscillators of the hypercube that lie directly on the boundary and successively the sets $\mathcal{L}_r$ of $(m-2r)^d - (m-2r-2)^d$ oscillators inside that are exactly r steps away from the surface of the hypercube. Starting from the set $\mathcal{L}_0$ and taking s steps on the lattice one can reach less than $(m+2s)^d - m^d$ oscillators outside the hypercube $m^{\times d}$. Therefore we find that the sum of all the elements of T that couple oscillators from the set $\mathcal{L}_0$ to oscillators outside the hypercube is bounded by $S_0 \leq 2\sum_{s=1}^{\infty}[(m+2s)^d - m^d]\frac{y^s}{1-y}$. Now consider the contribution from the set $\mathcal{L}_k$. Clearly, any oscillator outside the hypercube that can be reached from $\mathcal{L}_k$ in $s+k$ steps can be reached from $\mathcal{L}_0$ in s steps. Therefore, we can bound the sum S_k of all the elements of T that couple the set $\mathcal{L}_k$ to oscillators outside the hypercube by

$$S_k \leq 2\sum_{s=k+1}^{\infty}\{[m+2(s-k)]^d - m^d\}\frac{y^s}{1-y}.$$

As a consequence we obtain

$$E_N \leq \frac{2}{\sqrt{1-2cd}}\sum_{s=1}^{\infty}[(m+2s)^d - m^d]\frac{y^s}{1-y}\sum_{k=0}^{m/2}y^k.$$

Using the binomial expansion of $(m+2s)^d$ and the gamma function to bound expressions of the form $\sum_{s=0}^{\infty}y^s(2s)^k$, we find for $m > 4d/|\ln(y)|$ the bound

$$E_N \leq \frac{16d}{\sqrt{1-2cd}(1-2cd)^2|\ln(1-2cd)|^2}m^{d-1}, \quad (4)$$

which is the desired upper bound that is linear in the number of oscillators on the surface of the hypercube.

Lower bound.—In the following we demonstrate that the degree of entanglement, measured by the entropy of entanglement $E_{n,m}$, is asymptotically at least linear in the number of oscillators on the boundary between interior and exterior. The covariance matrix $\gamma_A = A \oplus D$ with nonincreasingly ordered symplectic eigenvalues $\mu_i = [\lambda_i(AD)]^{1/2}$ describes the reduced Gaussian state of the interior. Then

$$E_{n,m} = \sum_{i=1}^{m^d}\left(\frac{\mu_i+1}{2}\log\frac{\mu_i+1}{2} - \frac{\mu_i-1}{2}\log\frac{\mu_i-1}{2}\right)$$

depends only on the symplectic spectrum of the covariance matrix (see, e.g., Ref. [12]). The validity of the uncertainty relations [15] yields $\mu_i \geq 1$ for all $i = 1, \ldots, m^d$ so that

$$E_{n,m} \geq \sum_{i=1}^{m^d}\log[1+(\mu_i-1)] \geq \frac{\log\mu_1}{\mu_1-1}\sum_{i=1}^{m^d}(\mu_i-1).$$

To further bound the entropy we use that for any $k \geq 0$ and all $x \in [0,k]$ we have $\sqrt{1+x} \geq 1 + x(\sqrt{1+k}-1)/k$. Together with $\lambda_i(AD) = 1 + \lambda_i(-BE^{\mathrm{T}})$ and $\mu_i \geq 1$ we find

$$E_{n,m} \geq \frac{\log\mu_1}{\mu_1^2-1}\mathrm{tr}[-BE^{\mathrm{T}}] \geq \frac{1}{2\mu_1^2}\mathrm{tr}[-BE^{\mathrm{T}}].$$

By the Lidskii inequality [20] we then have $\lambda_1(AD) \leq \lambda_1(A)\lambda_1(D) \leq \lambda_1(\gamma_A)^2$, and from the pinching inequality [20], we find $\lambda_1(\gamma_A) \leq \lambda_1(\gamma)$. As before a discrete Fourier transform then yields $\lambda_1(\gamma) = (1-2cd)^{-1/2}$ so that μ_1 is bounded from below independently of m and n. All elements of B and $-E$ are positive. To bound these elements from below we start from $V^{\pm 1/2}$ as given above replacing the square root by its power series expansion in the parameter $2c$. We use $(1-x)^{1/2} = 1 - \sum_{s=1}^{\infty}B_s x^s$ as well as $B_j \geq 1/2^{j+1}$ and $\sum_{q=1}^{n}e^{2\pi ipq/n} = 0$ for integers p and q unless p is a multiple of n. Furthermore, we replace all multinomial coefficients by their trivial lower bound 1. Then the nondiagonal elements of $V^{1/2}$, and analogously $V^{-1/2}$, are bounded by $2|V_{\mathbf{k},\mathbf{l}}^{\pm 1/2}| \geq (c/2)^{s(\mathbf{k},\mathbf{l})}(1-c^2)^{-1}$. As a consequence we have $4\,\mathrm{tr}[-BE^{\mathrm{T}}] \geq \sum_{\mathbf{k},\mathbf{l}}(c/2)^{2s(\mathbf{k},\mathbf{l})}(1-c^2)^{-2}$. We can further bound this by considering only terms with $s(\mathbf{k},\mathbf{l}) = 1$ of which there are $2^d m^{d-1}$ so that

$$E_{n,m} \geq \frac{c^2\sqrt{1-2cd}}{16(1-c^2)^2}(2m)^{d-1}.$$

We thus obtain a lower bound proportional to the surface of the hypercube $m^{\times d}$. This concludes the proof.

In the following we briefly describe possible extensions of the above results that can be obtained by similar techniques, including more general interactions, thermal states, and classical correlations in classical systems.

Squared interactions.—The basic intuition behind the entanglement-area dependence becomes most transparent for the specific class of interactions for which the potential matrices V are of the form $V = W^2$ with a circulant band matrix W. In that case the covariance matrix of the ground state is given by $\gamma = W^{-1} \oplus W$. In this case one arrives at the connection between entanglement and area since one can show that (i) the number of terms contributing to the symplectic spectrum of the reduced covariance matrix is linear in the number of degrees of freedom at the boundary of the region and (ii) the respective symplectic eigenvalues are bounded from above and below independently of n and m. Note that property (i) is equivalent to the existence of a "disentangling" symplectic unitary transformation local to inside and outside of the regions such that only oscillators near to the boundary remain entangled. Taking, e.g., $V_1 = \mathrm{circ}(1+2c^2, -2c, c^2, 0, \ldots, c^2, -2c)$ (the case of nearest-neighbor and smaller next-to-nearest-neighbor interactions) allows one to show that only the oscillators exactly at the boundary contribute to the logarithmic negativity and that $\lambda_1(Q) \leq 2/(1-2c) - 1$, with Q being defined as in Eq. (3). For the same interaction in $d = 1$ spatial dimension one can even exactly calculate the symplectic spectrum of the reduced covariance matrix by means of a simple recursion relation. In the limit $m \to \infty$ this results in the two nonvanishing symplectic eigenvalues $\mu_1 = \mu_2 = (1 - c^2/q^2)^{-1/2}$, where $q = c + 1/2 \pm (c + 1/4)^{1/2}$.

Entanglement and area in classical systems.—It should be noted that, perhaps surprisingly, an area dependence can also be established analytically for classical correlations in classical harmonic lattice systems [16]. It is noteworthy that this result on classical systems can be established most economically using quantum techniques, namely, mapping the problem onto that of a quantum harmonic lattice with a squared interaction as has been described above.

Entanglement and area at finite temperature.—The property of squared interactions leading to effective disentanglement extends to thermal states and permits the proof of the linear entanglement-area dependence for finite temperatures. In that case operational entanglement measures such as the distillable entanglement are used. They can be bounded from below by the hashing inequality and from above again by the logarithmic negativity [16].

Summary and outlook.—For certain harmonic lattice Hamiltonians, e.g., discrete versions of the real Klein-Gordon field, we have proven analytically that the degree of entanglement between a hypercube and its environment can be bounded from above and below by expressions proportional to the number of degrees of freedom on the surface of the hypercube. This establishes rigorously a connection between entanglement and area in this system. Intuitively, this originates from the fact that one can approximately decouple the oscillators in the interior and the exterior up to a band of the width of the order of the correlation length of the system.

Our results can be extended to a wide variety of harmonic lattice Hamiltonians, both quantum and classical, and a future publication [16] will present details for more general interactions, both ground and thermal states and a careful discussion of the continuum limit, where the effective interaction strength is modified. Notably, in more general lattice systems, the exact relationship between an area dependence of the geometric entropy on the one hand and a nondivergent correlation length away from critical points on the other hand is still far from clear, even in one dimension. In particular, it is possible to consider critical systems in the sense of a divergent correlation length, yet keeping the above area dependence concerning the entanglement. It is our hope that the present Letter can stimulate further studies on such a general relationship between criticality and area dependence employing the insights and techniques that have been obtained in recent years in the development of a quantitative theory of entanglement in quantum information science.

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