# Entanglement and Criticality in Translationally Invariant Harmonic Lattice Systems with Finite-Range Interactions

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We discuss the relation between entanglement and criticality in translationally invariant harmonic lattice systems with nonrandom, finite-range interactions. We show that the criticality of the system as well as validity or breakdown of the entanglement area law are solely determined by the analytic properties of the spectral function of the oscillator system, which can easily be computed. In particular, for finite-range couplings we find a one-to-one correspondence between an area-law scaling of the bipartite entanglement and a finite correlation length. This relation is strict in the one-dimensional case and there is strong evidence for the multidimensional case. We also discuss generalizations to couplings with infinite range. Finally, to illustrate our results, a specific 1D example with nearest and next-nearest-neighbor coupling is analyzed.

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Because of the development of powerful tools to quantify entanglement, there is a growing interest in the relation between entanglement and criticality in quantum many-body systems. For a variety of spin models it was shown that in the absence of criticality, there is a strict relation between the von Neumann entropy of a compact subset of spins in the ground state and the surface area of the ensemble. For example, it was shown in [1–4] that the entanglement in noncritical one-dimensional spin chains approaches a constant value, while it grows logarithmically in the critical case, where the correlation length diverges. Employing field theoretical methods, it was argued that in $d$ dimensions the entropy grows as a polynomial of power $d-1$ under noncritical conditions, thus establishing an area theorem. A similar relation was suggested for harmonic lattice models in [5,6]. Very recently, employing methods of quantum information for Gaussian states, Plenio *et al.* [7] gave a derivation of the area theorem for harmonic lattice models with nearest-neighbor couplings. All these findings suggest a general correspondence between entanglement and criticality for nonrandom potentials. Yet recently special cases have been found for spin chains with Ising-type interactions [8] and for harmonic lattices systems [9] where the correlation length diverges but the entanglement obeys an area law. Thus the relation between entanglement scaling and criticality remains an open question. It should also be noted that in disordered systems, i.e., systems with random couplings the relation between entanglement area law and criticality is broken.

In this Letter we show that for harmonic lattice systems with *translational invariant*, *nonrandom*, and *finite-range* couplings, both entanglement scaling and criticality are determined by the analytic properties of the so-called spectral function. For finite-range interactions we find that the properties of the spectral function lead to a one-to-one correspondence between entanglement and criticality. To illustrate our results we discuss a specific one-dimensional example with nearest and next-nearest couplings. Despite the finite range of the coupling this model undergoes a transition from area-law behavior to unbounded logarithmic growth of entanglement.

Let us first consider a one-dimensional system, i.e., a chain of $N$ harmonic oscillators described by canonical variables $(q_i, p_i)$, $i = 1, 2, \ldots, N$. The oscillators are coupled by a translational invariant quadratic Hamiltonian

$$H = \frac{1}{2}\sum_{i=1}^{N} p_i^2 + \frac{1}{2}\sum_{i,j=1}^{N} V_{ij} q_i q_j, \tag{1}$$

where $V$ is a real, nonrandom, symmetric matrix with positive eigenvalues. For a translational invariant system $V$ is a Toeplitz matrix; i.e., its elements depend only on the difference of the indexes $V_{ij} \equiv V_k = V_{-k}$. For a finite system translational invariance implies furthermore periodic boundary conditions $V_k = V_{N-k}$. We assume in the following that the interactions are of finite range, i.e., that $V_k \equiv 0$ for $k \geq R$, where $R$ is a finite number independent on $N$. As we will show at the end of the Letter some generalizations to infinite range couplings are possible. Being positive definite, $V$ has a unique positive square root $V^{1/2}$ and its inverse $V^{-1/2}$, which completely determine the ground state in position (or momentum) representation, $\Psi_0(Q) \sim (\det V^{1/2})^{1/4} \exp\{-\frac{1}{4}\langle Q|V^{1/2}|Q\rangle\}$, [5,6].

The most important characteristic of the oscillator system is the spectrum of $V$. Since $V$ is a circulant matrix its eigenvalues can be expressed in terms of complex roots of unity $z_j = \exp\{i2\pi j/N\} = \exp\{i\theta_j\}$, $(j = 1, \ldots, N)$:

$$\lambda_j = \sum_{k=0}^{R-1} V_k (z_j)^k = \frac{1}{2}V_0 + \frac{1}{2}\sum_{k=-(R-1)}^{R-1} V_k (e^{i2\pi/Nj})^k. \tag{2}$$

Equation (2), together with the positivity of $V$, permits the representation $\lambda_j = h^2(z_j) = |h^2(z_j)|$, where $h(z_j)$ is a polynomial of order $(R-1)/2$ in $z_j$ (assuming for simplicity that $R$ is an odd number). Thus, $|h(z)| \sim \prod_{l=1}^{(R-1)/2} |z - \tilde{z}_l|$, where $\tilde{z}_l \equiv \exp\{i\alpha_l\}$ are the zeroth of $h(z)$ which are either real or complex conjugate pairs with $|\tilde{z}_l| \geq 1$ [10]. Let $Q \leq R$ be the number of real zeroth $\tilde{z}_r$ with multiplicity $m_r \in \{0, 1, \ldots\}$. Then, $\prod_{r=1}^{Q} |z_j - \tilde{z}_r|^{m_r} = \prod_{r=1}^{Q} [2 - 2\cos(\theta_j - \alpha_r)]^{m_r/2}$, and

$$\lambda(z_j) = \lambda_j = \lambda_0(z_j) \prod_{r=1}^{Q} [2 - 2\cos(\theta_j - \alpha_r)]^{m_r}. \quad (3)$$

$\lambda(z)$ is the so-called spectral function. $\lambda_0(z)$ is called the regular part of $\lambda$. It is a polynomial of the complex variable $z$ which has zeroth outside the unit circle. As a consequence, its inverse $\lambda_0^{-1}(z)$ is analytic on and inside the unit circle. $\prod_{r=1}^{Q} [2 - 2\cos(\theta - \alpha_r)]^{m_r}$ is called the singular part. If $\lambda$ is singular, i.e., if in the thermodynamic limit $V$ has eigenvalues arbitrarily close to zero, the total Hamiltonian, Eq. (1), has a vanishing energy gap between the ground and first excited state.

To evaluate sums of eigenvalues in the limit $N \to \infty$, one can interpret Eq. (2) as a Fourier series of $\lambda(\theta)$. Thus $V_k = \frac{1}{2\pi} \int_0^{2\pi} d\theta \lambda(\theta) \mathrm{e}^{-i\theta k}$. This integral representation is also valid for a finite number $N$ of oscillators up to an error $\mathcal{O}(1/N)$ as long as $k \leq (N+1)/2$. Because of the periodic boundary conditions $V^{\pm 1/2}$ are also Toeplitz matrices, and their elements $V_{ij}^{\pm 1/2} = V_k^{\pm 1/2}$ can be expressed in terms of $\lambda^{\pm 1/2}$ for $k \leq (N+1)/2$,

$$(V^{\pm 1/2})_k = \frac{1}{2\pi} \int_0^{2\pi} d\theta \lambda^{\pm 1/2}(\theta) \mathrm{e}^{-i\theta k}. \quad (4)$$

Since for the spatial correlation of an oscillator system holds $\langle q_i q_{i+l} \rangle \sim V_l^{-1/2}$ [11], the analytic properties of $\lambda^{-1/2}$ determine the spatial correlation length $\xi$:

$$\begin{aligned} \xi^{-1} &\equiv -\lim_{l\to\infty} \frac{1}{l} \ln|\langle q_i q_{i+l} \rangle| = -\lim_{l\to\infty} \frac{1}{l} \ln|V_l^{-1/2}| \\ &= -\lim_{l\to\infty} \frac{1}{l} \ln\left|\frac{1}{2\pi} \int_0^{2\pi} d\theta \lambda^{-1/2}(\theta) \mathrm{e}^{-i\theta l}\right|. \end{aligned} \quad (5)$$

If some derivative of $\lambda^{-1/2}(\theta)$, say the $m$th one, does not exist, partial integrations shows that the integral has a contribution proportional to $l^{-m}$. In this case the correlation length $\xi$ is infinite, defining a critical system. If, on the other hand, $\lambda^{-1/2}(\theta)$ is smooth the integral decays faster than any polynomial in $l^{-1}$. In this case the correlation length is finite, corresponding to a noncritical system. From the form of $\lambda(\theta)$ given in Eq. (3) it is clear that a regular spectral function implies a finite correlation length, i.e., a noncritical behavior and a singular one an infinite correlation length, i.e., a critical behavior.

In the following we will show that the analytic properties of $\lambda$ also determine the entanglement scaling of the oscillator system. The bipartite entanglement of a compact block of $N_1$ oscillators (inner partition $\mathcal{I}$) with the rest (outer partition $\mathcal{O}$) is determined by the $N_1$-dimensional submatrices $A$ and $D$ [5–7,11]

$$V^{-1/2} = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}, \qquad V^{1/2} = \begin{bmatrix} D & E \\ E^T & F \end{bmatrix}; \quad (6)$$

$C$ and $F$ are $(N - N_1) \times (N - N_1)$ matrices. The entropy is given by the eigenvalues $\mu_i \geq 1$ of the matrix product $AD$ [7]:

$$S = \sum_{i=1}^{N_1} f(\sqrt{\mu_i}), \quad (7)$$

where $f(x) = \frac{x+1}{2} \ln\frac{x+1}{2} - \frac{x-1}{2} \ln\frac{x-1}{2}$. Despite the simplicity of its form, (7) cannot be evaluated in general. This is in contrast to spin systems where $AD$ is itself a Toeplitz matrix [2,4].

An *upper bound* to $S$ can be found from the logarithmic negativity $\ln\|\rho^\Gamma\|$, where $\rho^\Gamma$ is the partial transpose of the total ground state $\rho$ and $\|\cdot\|$ denotes the trace norm. As shown in [7,9] the logarithmic negativity is bounded by the square root of the maximum eigenvalue of $V$ and a sum of absolute values of matrix elements of $V_{ij}^{-1/2}$ between all sites $i \in \mathcal{I}$ and $j \in \mathcal{O}$.

$$S \leq 4\lambda_{\max}^{1/2} \sum_{i\in\mathcal{I}} \sum_{j\in\mathcal{O}} |V_{ij}^{-1/2}|. \quad (8)$$

A *lower bound* to the entropy can be found making use of $\frac{x+1}{2} \ln\frac{x+1}{2} - \frac{x-1}{2} \ln\frac{x-1}{2} > \ln x$. This yields

$$S > \frac{1}{2} \sum_{i=1}^{N_1} \ln\mu_i = \frac{1}{2} \ln(\det AD). \quad (9)$$

This estimate has a simple and very intuitive meaning. To see this we first note that the matrix $D$ can be expressed in the form $D = [A - BC^{-1}B^\top]^{-1}$. Thus,

$$\begin{aligned} S &> -\frac{1}{2} \ln\det[(\mathbf{1} - BC^{-1}][B^T A^{-1}] \\ &= -\frac{1}{2} \ln\det\begin{pmatrix} A & B \\ B^T & C \end{pmatrix}\begin{pmatrix} A^{-1} & 0 \\ 0 & C^{-1} \end{pmatrix} \\ &= \frac{1}{2} \ln\frac{\det A \det C}{\det V^{-1/2}} = \frac{1}{2} \ln\frac{\det F \det D}{\det V^{1/2}}, \end{aligned} \quad (10)$$

where the last equation was obtained by expressing $A$ in terms of $D, E$, and $F$. The last line of (10) is just Shannon's classical mutual information $I(Q_1{:}Q_2)$ or $I(P_1{:}P_2)$, respectively, where $Q_1 = (q_1, q_2, \ldots, q_{N_1})$ and $Q_2 = (q_{N_1+1}, \ldots, q_N)$ are the position vectors of the two subsystems and $P_{1,2}$ the respective momentum vectors. $I(Q_1{:}Q_2)$ is defined as

$$I(Q_1{:}Q_2) = \int \mathrm{d}^N Q p(Q_1, Q_2) \ln\frac{p(Q_1, Q_2)}{p_1(Q_1) p_2(Q_2)}, \quad (11)$$

where $p(Q_1, Q_2) = |\Psi_0|^2$ is the total and $p_{1,2}(Q_{1,2})$ the reduced probability density in position space. Straightforward calculation shows

$$I(Q_1{:}Q_2) = \frac{1}{2}\ln\frac{(\det A)(\det C)}{\det V^{-1/2}} \leq S. \tag{12}$$

In order to evaluate Shannon's mutual information in the form given in Eq. (9) we want to make use of the asymptotic properties of Toeplitz matrices. For this we note that since $V^{\pm 1/2}$ are Toeplitz matrices, so are $A$ and $D$. Their elements $A_k$, and $D_k$ can be obtained from $\lambda^{\pm 1/2}$ by (4) if $N_1 \leq (N+1)/2$.

If $\lambda(\theta)$ is *regular*, we can apply the strong Szegö theorem [12], which states:

$$\det(D) \to \exp\left\{c_0 N_1 + \sum_{k=0}^{\infty} k|c_k|^2\right\}, \tag{13}$$

for $N_1 \to \infty$. Here the $c_k$ are Fourier coefficients of $\ln\lambda^{-1/2}(\theta)$, i.e., $c_k = \frac{1}{2\pi}\int_0^{2\pi} d\theta \ln\lambda^{1/2}(\theta)\mathrm{e}^{-i\theta k}$. Noting that the corresponding coefficients for $A$ have opposite sign, we find the lower bound

$$S \geq \frac{1}{2}\ln[\det(A)] + \frac{1}{2}\ln[\det(D)] = \sum_{k=0}^{\infty} k|c_k|^2. \tag{14}$$

To find an upper bound to $S$ we make use of Eq. (8). For a finite-range interaction there is always a maximum eigenvalue $\lambda_{\max}^{1/2}$. Furthermore, since $\lambda_0^{-1/2}(\theta)$ is smooth, Eq. (4) implies an exponential bound to the matrix elements of $V^{-1/2}$, i.e., $|V_{ij}^{-1/2}| \leq K\exp\{-\alpha|i-j|\}$, for $|i-j| \leq (N+1)/2$, where $K, \alpha > 0$. With this we find

$$\sum_{i\in\mathcal{I}}\sum_{j\in\mathcal{O}} |V_{ij}^{-1/2}| = 2N_1 \sum_{k=N_1+1}^{(N+1)/2} |V_k^{-1/2}| + 2\sum_{k=1}^{N_1} k|V_k^{-1/2}| < \frac{2K\mathrm{e}^{-\alpha}}{(1-\mathrm{e}^{-\alpha})^2}, \tag{15}$$

for $N, N_1 \to \infty$. Thus $S$ has also a finite upper bound in one dimension. One recognizes that for 1D harmonic chains with a *regular* spectral function $\lambda(\theta)$, the entropy has a lower and an upper bound independent on the number of oscillators, which implies an area theorem. Furthermore, as shown above, the spatial correlation length is finite, i.e., the system is noncritical.

Let us now consider a *singular* function $\lambda$. In this case we can calculate the asymptotic behavior of the Toeplitz determinants using Widom's theorem [13]. This theorem states that for $N_1 \to \infty$ and for $m_r > -1$,

$$\det D \to \exp\{c_0 N_1\} N_1^{\sum_r m_r^2/4}. \tag{16}$$

Widom's theorem cannot be applied to $A$, since $\lambda^{-1/2}(\theta) \sim \prod_r[2 - 2\cos(\theta - \alpha_r)]^{-m_r/2}$ involves negative exponents. We thus employ the alternative expression (11) containing the matrices $D$ and $F$. Since the elements of $D$ and $F$ can only be obtained by the Fourier transform (4) if their dimension is at most $(N+1)/2$, there is only one particular decomposition which we can consider, namely, $N_1 = (N-1)/2$ and $N_2 = (N+1)/2$. For the same reason it is not possible to apply Widom's theorem to $V^{1/2}$ as a whole. $\det V^{1/2}$ can, however, easily be calculated directly from the discrete eigenvalues (3). After a lengthy but straightforward calculation we eventually obtain the following expression for the mutual information with $N_1 = (N-1)/2$ and $N_2 = (N+1)/2$:

$$I = \left(\sum_{r=1}^{Q} \frac{m_r^2}{4}\right)\ln N + \text{const.} \tag{17}$$

Thus a singular spectral function $\lambda^{1/2}(\theta)$ in the case of half/half partitioning, leads to a lower bound to the entropy that grows logarithmically with the number of oscillators stating a breakdown of the area law of entanglement. As shown above, a singular spectral function also implies a diverging spatial correlation length, defining a critical system.

The above discussion can be extended to $d$ dimensions. In this case, one would consider the entropy $S$ of a hypercube of oscillators with dimensions $N_1 \times N_2 \times \cdots \times N_d$. Since we are interested in the thermodynamic limit we can again assume $N_i \leq (N+1)/2$. In this case, the matrices $A$ and $D$ are Toeplitz matrices with respect to each spatial direction and their elements $A_{k_1,k_2,\ldots,k_d}$ can be obtained from the square root of the $d$-dimensional function $\lambda(\theta_1,\ldots,\theta_d) = \sum_{k_1=0}^{N_1-1}\ldots\sum_{k_d=0}^{N_d-1} V_{k_1,\ldots,k_d}\exp\{i\sum_{j=1}^{d}\theta_j k_j\}$. If $\lambda^{1/2}$ is *regular*, the $d$-dimensional Szegö theorem holds [14], which asserts that the Toeplitz determinant of dimension $n_1 \times n_2 \times \cdots \times n_d$ has the asymptotic form

$$\det D \to \exp\left\{c_0 n_1 \cdots n_d + \sum_{j=1}^{d} \frac{n_1 \cdots n_d}{n_j}|C_j|\right\}, \tag{18}$$

where $c_0 = \frac{1}{(2\pi)^d}\int_0^{2\pi} d\theta_1 \cdots \int_0^{2\pi} d\theta_d \ln[\lambda^{1/2}(\theta_1,\ldots,\theta_d)]$, and the $C_i$ are some constants, whose explicit form is of no interest here. We see that under the above conditions for the $d$-dimensional characteristic function $\lambda^{1/2}(\theta_1,\ldots,\theta_d)$ the entropy has the lower bound

$$S > \sum_{j=1}^{d} \frac{n_1 n_2 \cdots n_d}{n_j} C_j \sim n^{d-1}, \tag{19}$$

which is again proportional to the surface area. We note that the lower bound (19) to the entropy given by the multidimensional Szegö theorem is more general than the estimates given in [7,9], which are restricted to nearest-neighbor interactions. From the exponential bound to the matrix elements of $V^{-1/2}$ one can also find an upper bound to the entropy using Eq. (8):

$$\sum_{i\in\mathcal{I}}\sum_{j\in\mathcal{O}} |V_{ij}^{-1/2}| \leq K\sum_{j=1}^{d} \frac{n_1 n_2 \cdots n_d}{n_j} \sim n^{d-1}. \tag{20}$$

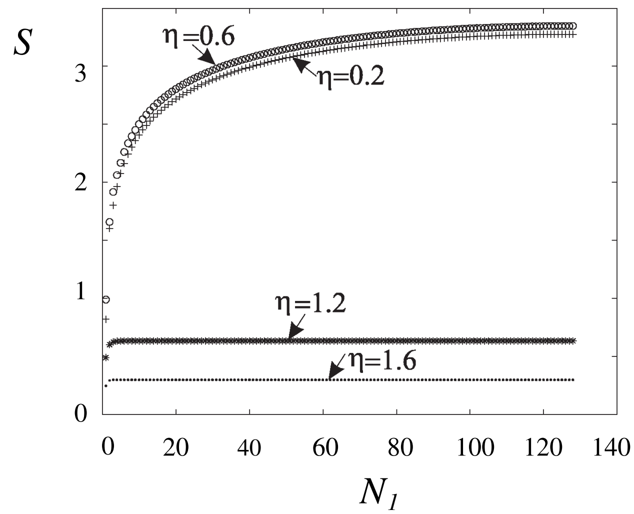


FIG. 1. Entropy as function of partition size for a noncritical ($\eta = 1.2, 1.6$) and critical harmonic chain ($\eta = 0.2, 0.6$) for the example of the text obtained from numerical calculation of Eq. (7).

Eqs. (19) and (20) establish an area law for arbitrary dimensions in the case of a regular spectral function.

In order to obtain a lower bound to the entropy for a *singular* spectral function in more than one dimension and to show a corresponding breakdown of the entanglement area law, one would need a multidimensional generalization of Widom's theorem [13]. Although no such generalization is known to us, there is strong evidence for a breakdown of the area law in higher dimensions. First of all, for an interaction matrix that is separable in the $d$ dimensions, i.e., whose elements can be written as products $V_{i_1,j_1}V_{i_2,j_2}\dots V_{i_d,j_d}$, the 1D discussion can be straightforwardly extended to $d$ dimensions. Second, Widom has given a generalization of his matrix theorem to operator functions $f(A)$ on $R^d$ [15]. The proof given in [15] makes, however, use of strong conditions on $f$ that are not fulfilled for the case we are interested in here.

To illustrate validity and breakdown of the area theorem let us consider the Hamiltonian $H = \frac{1}{2}\sum_{i=1}^N p_i^2 + \frac{1}{2} \times \sum_{i=1}^N(-2\eta q_i + q_{i+1} + q_{i-1})^2$ with periodic boundary conditions. The square root of the spectral function reads in this case $\lambda^{1/2}(\theta) = |2\eta - 2\cos\theta|$. For $\eta > 1$, $\lambda^{1/2}$ is regular and the correlation length is finite. For $\eta < 1$, $\lambda^{1/2}(\theta)$ can be written as $\lambda^{1/2}(\theta) = [2 - 2\cos(\theta + \theta_0)]^{1/2}[2 - 2\cos(\theta - \theta_0)]^{1/2}$, with $\eta = \cos\theta_0$, and thus is singular. In this case the correlation length is infinite. We have numerically calculated the entropy for this system for different values of $\eta$. The results are shown in Fig. 1. One recognizes an unlimited logarithmic growth of $S$ for $\eta < 1$ and a saturation for $\eta > 1$.

In the present Letter we discussed the relation between entanglement and criticality in translational invariant harmonic lattice systems with finite-range couplings. We have shown that upper and lower bounds to the entropy of entanglement as well as the correlation length are solely determined by the analytic properties of the spectral function. If the spectral function is regular, the entanglement obeys an area law and the system is noncritical. If the spectral function has a singular part, the area law breaks down and the system is critical. Thus for harmonic lattice systems with *translational invariant*, *nonrandom*, and *finite-range* couplings there is a one-to-one correspondence between entanglement and criticality. We note that some of our results apply also to more general couplings. For the estimates of the entropy it is sufficient that the number of roots of $h(z)$ on the unit circle is finite. This is always fulfilled for banded coupling matrices $V$ but also holds under more general conditions. For couplings of infinite range, the regular part of the spectral function $\lambda_0$ is no longer a polynomial. Thus $\lambda_0^{-1/2}$ may not be smooth anymore and could have a singularity in a derivative of some order. In such a case the spectral function could be regular, allowing for an entanglement area theorem, and at the same time the correlation length would be infinite; i.e., the system would be critical as in the example of Ref. [9].

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