Quantum States on Harmonic Lattices

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Abstract: We investigate bosonic Gaussian quantum states on an infinite cubic lattice in arbitrary spatial dimensions. We derive general properties of such states as ground states of quadratic Hamiltonians for both critical and non-critical cases. Tight analytic relations between the decay of the interaction and the correlation functions are proven and the dependence of the correlation length on band gap and effective mass is derived. We show that properties of critical ground states depend on the gap of the point-symmetrized rather than on that of the original Hamiltonian. For critical systems with polynomially decaying interactions logarithmic deviations from polynomially decaying correlation functions are found.

1. Introduction

The importance of bosonic Gaussian states arises from two facts. First, they provide a very good description for accessible states of a large variety of physical systems. In fact, every ground and thermal state of a quadratic bosonic Hamiltonian is Gaussian and remains so under quadratic time evolutions. In this way quadratic approximations naturally lead to Gaussian states. Hence, they are ubiquitous in quantum optics as well as in the description of vibrational modes in solid states, ion traps or nanomechanical oscillators.

The second point for the relevance of Gaussian states is that they admit a powerful phase space description which enables us to solve quantum many-body problems which are otherwise (e.g., for spin systems) hardly tractable. In particular, the phase space dimension, and with it the complexity of many tasks, scales linearly rather than exponentially in the number of involved subsystems. For this reason quadratic Hamiltonians and the corresponding Gaussian states also play a paradigmatic role as they may serve as an exactly solvable toy model from which insight into other quantum systems may be gained.

Exploiting the symplectic tools of the phase space description, exact solutions have been found for various problems in quantum information theory as well as in quantum

statistical mechanics. In fact, many recent works form a bridge between these two fields as they address entanglement questions for asymptotically large lattices of quadratically coupled harmonic oscillators: the entropic area law [1–3] has been investigated as well as entanglement statics [4–6], dynamics [7–9] and frustration [10, 11].

In the present paper we analytically derive general properties of ground states of translationally invariant quadratic Hamiltonians on a cubic lattice. We start by giving an outlook and a non-technical summary of the main results. The results on the asymptotic scaling of ground state correlations are summarized in Table 1.

We note that related investigations of correlation functions were recently carried out in [12, 13] for finite dimensional spin systems and in [1, 14] for generic harmonic lattices with non-critical finite range interactions.

Quadratic Hamiltonians. In Sect. 2, we start by introducing some basic results on quadratic Hamiltonians together with the used notation.

Translationally invariant systems. In Sect. 3, we show first that every pure translational invariant Gaussian state is point symmetric. This implies that the spectral gap of the symmetrized rather than the original Hamiltonian determines the characteristic properties of the ground state. We provide a general formula for the latter and express its covariance matrix in terms of a product of the inverse of the Fourier transformed spectral function and the Hamiltonian matrix.

Non-critical systems. Section 4 shows that if the Hamiltonian is gapped, then the correlations decay according to the interaction: a (super) polynomial decay of the interaction leads to the same (super) polynomial decay for the correlations, and (following Ref. [1]) finite range interactions lead to exponentially decaying correlations.

Correlation length and gap. Section 5 gives an explicit formula for the correlation length for gapped 1D-Hamiltonians with finite range interactions. The correlation length ξ is expressed in terms of the dominating zero of the complex spectral function, which close

interaction	non-critical	critical
local	$O^*(e^{-n/\xi})$ $d = 1: \xi \sim \frac{1}{\sqrt{\Delta m^*}} = \frac{v}{\Delta}$	$d = 1: O^*\left(\frac{1}{n^2}\right)$ $d > 1: O\left(\frac{\log n}{n}\right)$
$O(n^{-\infty})$	$O(n^{-\infty})$	
$O\left(\frac{1}{n^{\alpha}}\right)$	$O\left(\frac{1}{n^{\nu-d}}\right)$	(nd+1)
$\alpha > 2d + 1$	$\alpha > \nu \in \mathbb{N}$	
$\frac{c}{n^{\alpha}}$ $d = 1$	$\alpha \ge 2: \Theta\left(\frac{1}{n^{lpha}}\right)$	$\alpha = 3: \begin{cases} \Theta(\frac{1}{n^2}) , c > 0\\ \Theta(\frac{\sqrt{\log n}}{n^2}), c < 0\\ \alpha > 3: \Theta(\frac{1}{n^2}) \end{cases}$

Table 1. Summary of the bounds derived in the paper on the asymptotic scaling of ground state correlations, depending on the scaling of the interaction (left column). Here *n* is the distance between two points (harmonic oscillators) on a cubic lattice of dimension *d*. *O* denotes upper bounds, O^* tight upper bounds, and Θ the exact asyptotics. The table shows the results for generic interactions—special cases are discussed in the text

to a critical point is in turn determined by the spectral gap Δ and the effective mass m^* at the band gap via $\xi \sim (m^* \Delta)^{-1/2}$. When the change in the Hamiltonian is given by a global scaling of the interactions this proves the folk theorem $\xi \sim 1/\Delta$.

Critical systems. Section 6 shows that for generic *d*-dimensional critical systems the correlations decay as $1/n^{d+1}$, where *n* is the distance between two points on the lattice. Whereas for sufficiently fast decreasing interactions in d = 1 the asymptotic bound is exactly polynomial, it contains an additional logarithmic correction for $d \ge 2$. Similarly for d = 1 a logarithmic deviation is found if the interaction decays exactly like $-1/n^3$.

2. Quadratic Hamiltonians and their Ground States

Consider a system of N bosonic modes which are characterized by N pairs of canonical operators $(Q_1, P_1, \ldots, Q_N, P_N) =: R$. The canonical commutation relations (CCR) are governed by the symplectic matrix σ via

$$\begin{bmatrix} R_k, R_l \end{bmatrix} = i\sigma_{kl}, \quad \sigma = \bigoplus_{n=1}^N \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

and the system may be equivalently described in terms of bosonic creation and annihilation operators $a_l = (Q_l + i P_l)/\sqrt{2}$. Quadratic Hamiltonians are of the form

$$\mathcal{H}=\frac{1}{2}\sum_{kl}H_{kl}R_kR_l,$$

where the Hamiltonian matrix H is real and positive semidefinite due to the Hermiticity and lower semi-boundedness of the Hamiltonian \mathcal{H} . Without loss of generality we neglect linear and constant terms since they can easily be incorporated by a displacement of the canonical operators and a change of the energy offset. Before we discuss the general case we mention some important special instances of quadratic Hamiltonians: a well studied 1D example of this class is the case of nearest neighbor interactions in the position operators of harmonic oscillators on a chain with periodic boundary conditions

$$\mathcal{H}_{\kappa} = \frac{1}{2} \sum_{i=1}^{N} Q_i^2 + P_i^2 - \kappa \ Q_i Q_{i+1} , \quad \kappa \in [-1, 1].$$
(1)

This kind of spring-like interaction was studied in the context of information transfer [7], entanglement statics [4–6] and entanglement dynamics [9]. Moreover, it can be considered as the discretization of a massive bosonic continuum theory given by the Klein-Gordon Hamiltonian

$$\mathcal{H}_{\rm KG} = \frac{1}{2} \int_{-L/2}^{L/2} \left[\dot{\phi}(x)^2 + \left(\nabla \phi(x) \right)^2 + m^2 \phi(x)^2 \right] dx,$$

where the coupling κ is related to the mass m by $\kappa^{-1} = 1 + \frac{1}{2} \left(\frac{mL}{N}\right)^2$ [5]. Other finite range quadratic Hamiltonians appear as limiting cases of finite range spin Hamiltonians via the Holstein–Primakoff approximation [15]. In this way the xy-spin model with transverse magnetic field can for instance be mapped onto a quadratic bosonic Hamiltonian in the limit of strong polarization where $a \simeq (\sigma_x + i\sigma_y)/2$. Longer range interactions appear naturally for instance in 1D systems of trapped ions. These can either be implemented as

Coulomb crystals in Paul traps or in arrays of ion microtraps. When expanding around the equilibrium positions, the interaction between two ions at position *i* and $j \neq i$ is in harmonic approximation—of the form $\frac{c Q_i Q_j}{|i-j|^3}$, where c > 0 (c < 0) if Q_i , Q_j are position operators in radial (axial) direction [16].

Let us now return to the general case and briefly recall the normal mode decomposition [17]: every Hamiltonian matrix can be brought to a diagonal normal form by a congruence transformation with a symplectic matrix $S \in \text{Sp}(2N, \mathbb{R}) = \{S | S\sigma S^T = \sigma\}$:¹

$$SHS^{T} = \bigoplus_{i=1}^{I} \begin{pmatrix} \varepsilon_{i} & 0\\ 0 & \varepsilon_{i} \end{pmatrix} \oplus \bigoplus_{j=1}^{J} \begin{pmatrix} 0 & 0\\ 0 & 1 \end{pmatrix}, \quad \varepsilon_{i} > 0,$$
(2)

where the symplectic eigenvalues ε_i are the square roots of the duplicate nonzero eigenvalues of $\sigma H \sigma^T H$. The diagonalizing symplectic transformation S has a unitary representation U_S on Hilbert space which transforms the Hamiltonian according to

$$U_{S}\mathcal{H}U_{S}^{\dagger} = \frac{1}{2}\sum_{i=1}^{I} \left(Q_{i}^{2} + P_{i}^{2}\right)\varepsilon_{i} + \frac{1}{2}\sum_{j=1}^{J}P_{j}^{2} = \sum_{i=1}^{I} \left(a_{i}^{\dagger}a_{i} + \frac{1}{2}\right)\varepsilon_{i} + \frac{1}{2}\sum_{j=1}^{J}P_{j}^{2}.$$
 (3)

Hence, by Eq. (3) the ground state energy E_0 and the energy gap Δ can easily be expressed in terms of the symplectic eigenvalues of the Hamiltonian matrix:

$$E_0 = \frac{1}{2} \sum_{i=1}^{I} \varepsilon_i, \quad \Delta = \begin{cases} \min_i \varepsilon_i, \ J = 0\\ 0, \qquad J > 0 \end{cases}.$$
(4)

The case of a vanishing energy gap $\Delta = 0$ is called *critical* and the respective ground states are often qualitatively different from those of non-critical Hamiltonians. For the Hamiltonian \mathcal{H}_{κ} , Eq. (1), this happens in the strong coupling limit $|\kappa| = 1 - \Delta^2 \rightarrow 1$, and in the case of 1D Coulomb crystals a vanishing energy gap in the radial modes can be considered as the origin of a *structural phase transition* where the linear alignment of the ions becomes unstable and changes to a zig-zag configuration [18–20]. Needless to say, these phase transitions appear as well in higher dimensions and for various different configurations [21].

Ground and thermal states of quadratic Hamiltonians are *Gaussian states*, i.e, states having a Gaussian Wigner distribution in phase space. In the mathematical physics literature they are known as bosonic *quasi-free states* [22, 23]. These states are completely characterized by their first moments $d_k = tr[\rho R_k]$ (which are w.l.o.g. set to zero in our case) and their *covariance matrix* (CM)

$$\gamma_{kl} = \operatorname{tr} \Big[\rho \big\{ R_k - d_k, R_l - d_l \big\}_+ \Big], \tag{5}$$

where $\{\cdot, \cdot\}_+$ is the anticommutator. The CM satisfies $\gamma \ge i\sigma$, which expresses Heisenberg's uncertainty relation and is equivalent to the positivity of the corresponding density operator $\rho \ge 0$. In order to find the ground state of a quadratic Hamiltonian, observe that

$$\frac{1}{2}\sum_{i}\varepsilon_{i} \stackrel{(4)}{=} E_{0} = \inf_{\rho} \operatorname{tr}[\rho\mathcal{H}] \stackrel{(5)}{=} \frac{1}{4}\inf_{\gamma} \operatorname{tr}[\gamma\mathcal{H}].$$
(6)

¹ Note that we disregard systems where the Hamiltonian contains irrelevant normal modes.

By virtue of Eqs. (2,3) the infimum is attained for the ground state covariance matrix

$$\gamma = \lim_{s \to \infty} S^T \left[\bigoplus_{i=1}^{I} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \oplus \bigoplus_{j=1}^{J} \begin{pmatrix} s & 0 \\ 0 & s^{-1} \end{pmatrix} \right] S, \tag{7}$$

which reduces to $\gamma = S^T S$ in the non-critical case. Note that the ground state is unique as long as *H* does not contain irrelevant normal modes [which we have neglected from the very beginning in Eq. (2)].

In many cases it is convenient to change the order of the canonical operators such that $R = (Q_1, \ldots, Q_N, P_1, \ldots, P_N)$. Then the covariance matrix as well as the Hamiltonian matrix can be written in block form

$$H = \begin{pmatrix} H_Q & H_{QP} \\ H_{QP}^T & H_P \end{pmatrix}.$$

In this representation a quadratic Hamiltonian is particle number preserving iff $H_Q = H_P$ and $H_{QP} = -H_{QP}^T$, that is, the Hamiltonian contains only terms of the kind $a_i^{\dagger}a_j + a_j^{\dagger}a_i$. In quantum optics terms of the form $a_i^{\dagger}a_j^{\dagger}$, which are not number preserving, are neglected within the framework of the *rotating wave approximation*. The resulting Hamiltonians have particular simple ground states:

Theorem 1a. The ground state of any particle number preserving Hamiltonian is the vacuum with $\gamma = 1$, and the corresponding ground state energy is given by $E_0 = \frac{1}{4} \operatorname{tr} H$.

Proof. Number preserving Hamiltonians are most easily expressed in terms of creation and annihilation operators. For this reason we change to the respective complex representation via the transformation

$$H \mapsto \Omega H \Omega^T = \begin{pmatrix} 0 & X \\ \bar{X} & 0 \end{pmatrix}, \quad \Omega = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & -i\mathbb{1} \\ \mathbb{1} & i\mathbb{1} \end{pmatrix}.$$

In this basis *H* is transformed to normal form via a block diagonal unitary transformation $U \oplus \overline{U}$ which in turn corresponds to an element of the orthogonal subgroup of the symplectic group $\operatorname{Sp}(2N, \mathbb{R}) \cap \operatorname{SO}(2N) \simeq \operatorname{U}(N)$ [24]. Hence, the diagonalizing *S* in Eqs. (2,7) is orthogonal and since J = 0 due to particle number conservation, we have $\gamma = S^T S = \mathbb{1}$. E_0 follows then immediately from Eq. (6). \Box

Another important class of quadratic Hamiltonians for which the ground state CM takes on a particular simple form corresponds to the case $H_{QP} = 0$ where there is no coupling between the momentum and position operators:

Theorem 1b. For a quadratic Hamiltonian with Hamiltonian matrix $H = H_Q \oplus H_P$ the ground state energy and the ground state CM are given by

$$E_0 = \frac{1}{2} \text{tr} \left[\sqrt{H_Q} \sqrt{H_P} \right], \quad \gamma = X \oplus X^{-1}, \quad X = H_Q^{-1/2} \sqrt{H_Q^{1/2} H_P H_Q^{1/2}} H_Q^{-1/2}.$$
(8)

Proof. Since $\sigma H \sigma^T H = H_P H_Q \oplus H_Q H_P$, the symplectic eigenvalues of H are given by the eigenvalues of $\sqrt{H_Q}\sqrt{H_P}$ and thus $E_0 = \frac{1}{2} \text{tr} [\sqrt{H_Q}\sqrt{H_P}]$. Moreover, by the uniqueness of the ground state and the fact that $E_0 = \frac{1}{4} \text{tr} [\gamma H]$ with γ from Eq. (8) we know that γ is the ground state CM (as it is an admissible pure state CM by construction). Finally we give a general formula for the ground state CM in cases where the blocks in the Hamiltonian matrix can be diagonalized simultaneously. This is of particular importance as it applies to all translational invariant Hamiltonians discussed in the following sections.

Theorem 1c. Consider a quadratic Hamiltonian for which the blocks H_Q , H_P , H_{QP} of the Hamiltonian matrix can be diagonalized simultaneously and in addition $H_{QP} = H_{QP}^T$. Then with

$$\hat{\mathcal{E}} = \sqrt{H_Q H_P - H_{QP}^2} \quad we have \tag{9}$$

$$E_0 = \frac{1}{2} \operatorname{tr}[\hat{\mathcal{E}}], \quad \Delta = \lambda_{\min}(\hat{\mathcal{E}}), \quad \gamma = (\hat{\mathcal{E}} \oplus \hat{\mathcal{E}})^{-1} \sigma H \sigma^T.$$
(10)

Proof. Since $\sigma H \sigma^T H = \hat{\mathcal{E}}^2 \oplus \hat{\mathcal{E}}^2$ we have indeed $E_0 = \frac{1}{2} \text{tr}[\hat{\mathcal{E}}]$ and $\Delta = \lambda_{\min}(\hat{\mathcal{E}})$. Positivity $\gamma \ge 0$ is implied by $H \ge 0$ such that we can safely talk about the symplectic eigenvalues of γ . The latter are, however, all equal to one due to $(\gamma \sigma)^2 = -\mathbb{1}$ so that γ is an admissible pure state CM. Moreover it belongs to the ground state since $\frac{1}{4} \text{tr}[H\gamma] = E_0$. \Box

3. Translationally Invariant Systems

Let us now turn towards translationally invariant systems. We consider cubic lattices in *d* dimensions with periodic boundary conditions. For simplicity we assume that the size of the lattice is N^d . The system is again characterized by a Hamiltonian matrix H_{kl} , where the indices k, l, which correspond to two points (harmonic oscillators) on the lattice, are now *d*-component vectors in \mathbb{Z}_N^d . Translational invariance is then reflected by the fact that any matrix element $A_{kl}, A \in \{H_Q, H_P, H_{QP}\}$ depends only on the relative position k - l of the two points on the lattice, and we will therefore often write $A_{k-l} = A_{kl}$. Note that due to the periodic boundary conditions k - l is understood modulo N in each component. Matrices of this type are called *circulant*, and they are all simultaneously diagonalized via the Fourier transform

$$\mathcal{F}_{\alpha\beta} = \frac{1}{\sqrt{N}} e^{\frac{2\pi i}{N}\alpha\beta}, \quad \alpha, \beta \in \mathbb{Z}_N, \quad \text{such that}$$
$$\hat{A} := \mathcal{F}^{\otimes d} A \mathcal{F}^{\dagger \otimes d} = \text{diag} \left(\sum_{n \in \mathbb{Z}_N^d} A_n \ e^{-\frac{2\pi i}{N}mn} \right)_m$$

where mn is the usual scalar product in \mathbb{Z}_N^d . It follows immediately that all circulant matrices mutually commute.

In the following, we will show that we can without loss of generality restrict ourselves to point-symmetric Hamiltonians, i.e., those for which $H_{QP} = H_{QP}^T$ (which means that \mathcal{H} contains only pairs $Q_k P_l + Q_l P_k$). For dimension d = 1 this is often called reflection symmetry.

Theorem 2. Any translationally invariant pure state CM Γ is point symmetric.

Proof. For the proof, we use that any pure state covariance matrix can be written as

$$\Gamma = \begin{pmatrix} \Gamma_Q & \Gamma_{QP} \\ \Gamma_{QP}^T & \Gamma_P \end{pmatrix} = \begin{pmatrix} X & XY \\ YX & X^{-1} + YXY \end{pmatrix},$$

where $X \ge 0$ and *Y* is real and symmetric [25]. From translational invariance, it follows that all blocks and thus *X* and *Y* have to be circulant and therefore commute. Hence, $\Gamma_{QP} = XY = YX = \Gamma_{QP}^{T}$, i.e., Γ is point symmetric. \Box

Let $\mathcal{P}: \mathbb{Z}_N^d \to \mathbb{Z}_N^d$ be the reflection on the lattice and define the symmetrization operation $\mathcal{S}(A) = \frac{1}{2}(A + \mathcal{P}A\mathcal{P})$ such that by the above theorem $\mathcal{S}(\gamma) = \gamma$ for every translational invariant pure state CM. Then due to the cyclicity of the trace we have for any translational invariant Hamiltonian

$$\inf_{\gamma} \operatorname{tr} \big[H\gamma \big] = \inf_{\gamma} \operatorname{tr} \big[\mathcal{S}(H)\gamma \big].$$

Hence, the point-symmetrized Hamiltonian S(H), which differs from H by the offdiagonal block $S(H_{QP}) = \frac{1}{2}(H_{QP} + H_{QP}^T)$ has both the same ground state energy and the same ground state as H. Together with Theorem 1c this leads us to the following:

Theorem 3. Consider any translationally invariant quadratic Hamiltonian. With $\hat{\mathcal{E}} = \left[H_Q H_P - \frac{1}{4}(H_{QP} + H_{QP}^T)^2\right]^{1/2}$ the ground state CM and the corresponding ground state energy are given by

$$E_0 = \frac{1}{2} \text{tr}[\hat{\mathcal{E}}], \quad \gamma = \left(\hat{\mathcal{E}} \oplus \hat{\mathcal{E}}\right)^{-1} \sigma \mathcal{S}(H) \sigma^T.$$
(11)

It is important to note that the energy gaps of H and $\mathcal{S}(H)$ will in general be different. In particular H might be gapless while $\mathcal{S}(H)$ is gapped. However, as we will see in the following sections, the properties of γ depend on the gap $\Delta = \lambda_{\min}(\hat{\mathcal{E}})$ of the symmetrized Hamiltonian rather than on that of the original H. For this reason we will in the following for simplicity assume $H_{QP} = H_{QP}^T$. By Thm. 3 all results can then also be applied to the general case without point symmetry if one only keeps in mind that Δ is the gap corresponding to $\mathcal{S}(H)$.

Note that the eigenvalues of $\hat{\mathcal{E}}$ are the symplectic eigenvalues of $\mathcal{S}(H)$, i.e., $\mathcal{E} = \mathcal{F}^{\otimes d} \hat{\mathcal{E}} \mathcal{F}^{\dagger \otimes d}$ is the excitation spectrum of the Hamiltonian. This is the reason for the notation where \mathcal{E} resides in Fourier space and $\hat{\mathcal{E}}$ in real space, which differs from the normal usage of the hat throughout the paper.

Correlation functions. According to Eqs. (9,10,11) we have to compute the entries of functions of matrices in order to learn about the entries of the covariance matrix. This is most conveniently done by a double Fourier transformation, where one uses that $\widehat{f(M)} = f(\hat{M})$, and we find

$$[f(M)]_{nm} = \frac{1}{N^d} \sum_{r,s} e^{-\frac{2\pi i}{N} nr} [f(\hat{M})]_{rs} e^{\frac{2\pi i}{N} sm}.$$
 (12)

As we consider translationally invariant systems, M is circulant and thus \hat{M} is diagonal. We define the function

$$\hat{M}(\phi) = \sum_{n \in \mathbb{Z}_N^d} M_n \, e^{-in\phi} \tag{13}$$

such that $\hat{M}(2\pi r/N) = \hat{M}_{r,r}$. As f(M) is solely determined by its first row, we can write

$$[f(M)]_n = \frac{1}{N^d} \sum_{r \in \mathbb{Z}_N^d} e^{2\pi i \, nr/N} f(\hat{M}(2\pi r/N)).$$
(14)

In the following we will use the index $n \in \mathbb{Z}^d$ for the relative position of two points on the lattice. Their distance will be measured either by the l_1, l_2 or l_{∞} norm. Since we are considering finite dimensional lattices these are all equivalent for our purpose and we will simply write ||n||. In the thermodynamic limit $N \to \infty$, the sum in Eq. (14) converges to the integral

$$[f(M)]_n = \frac{1}{(2\pi)^d} \int_{\mathcal{T}^d} \mathrm{d}\phi \ f(\hat{M}(\phi)) \ e^{in\phi} \quad \text{with} \quad \hat{M}(\phi) = \sum_{n \in \mathbb{Z}^d} M_n \ e^{-in\phi}, \quad (15)$$

where \mathcal{T}^d is the *d*-dimensional torus, i.e., $[0, 2\pi]^d$ with periodic boundary conditions. The convergence holds as soon as $\sum |M_n| < \infty$ [which holds e.g. for $M_n = O(||n||^{-\alpha})$] with some $\alpha > d$] and f is continuous on an open interval which contains the range of \hat{M} .

From the definition (15) of \hat{M} , it follows that $\hat{M} \in \mathscr{C}^k(\mathcal{T}^d)$ (the *n* times continuously differentiable functions on \mathcal{T}^d) whenever the entries M_n decay at least as fast as $||n||^{-\alpha}$ for some $\alpha > k + d$, since then the sum of the derivatives converges uniformly. Particularly, if the entries of M decay faster than any polynomial, then $\hat{M} \in \mathscr{C}^{\infty}(\mathcal{T}^d)$. In the following the most important function of the type $f \circ \hat{M}$ will be the spectral function

$$\mathcal{E}(\phi) = \sqrt{\sum_{n \in \mathbb{Z}^d} e^{-in\phi} \left([H_Q H_P]_n - [H_{QP}^2]_n \right)}.$$
(16)

Asymptotic notation. As the main issue of this paper is the asymptotic scaling of correlations, we use the Landau symbols o, O, and Θ , as well as the symbol O^{*} for tight bounds:

- f(x) = o(g(x)) means $\lim_{x \to \infty} \frac{f(x)}{g(x)} = 0$, i.e., f vanishes strictly faster than g for $x \to \infty;$
- f(x) = O(g(x)), if $\limsup_{x \to \infty} \left| \frac{f(x)}{g(x)} \right|$ is finite, i.e., f vanishes at least as fast as g; $f(x) = \Theta(g(x))$, if f(x) = O(g(x)) and g(x) = O(f(x)) (i.e., exact asymptotics);
- $f(x) = O^*(g(x))$, if f(x) = O(g(x)) but $f(x) \neq o(g(x))$, i.e., g is a tight bound on f^{2} If f is taken from a set (e.g., those functions consistent with the assumptions of a theorem) we will write $f = O^*(g)$ if g is a tight bound for at least one f (i.e., the best possible universal bound under the given assumptions).

If talking about Hamiltonians, the scaling is meant to hold for all blocks, e.g., if the interaction vanishes as $O(||n||^{-\alpha})$ for $n \to \infty$, this holds for all the blocks H_Q , H_P , and $H_{QP} = H_{PQ}^{T}$. The same holds for covariance matrices in the non-critical case. By the shorthand notation $f(n) = o(||n||^{-\infty})$, we mean that $f(n) = o(||n||^{-\alpha}) \forall \alpha > 0$. Note finally that the Landau symbols are also used in (Taylor) expansions around a point x_0 where the considered limit is $x \to x_0$ rather than $x \to \infty$.

4. Non-Critical Systems

In this section, we analyze the ground state correlations of non-critical systems, i.e., those which exhibit an energy gap $\Delta > 0$ between the ground and the first excited state.

² In order to see the difference to Θ , take an f(x) = g(x) for even x, f(x) = 0 for odd $x, x \in \mathbb{N}$. Although f does not bound g, thus $f(x) \neq O(g(x))$, the bound g is certainly tight. A situation like this is met, e.g., in Theorem 5, where the correlations oscillate within an exponentially decaying envelope.

Simply speaking, we will show that the decay of correlations reflects the decay of the interaction. While local (super-polynomially decaying) interactions imply exponentially (super-polynomially) decaying correlations, a polynomial decay of interactions will lead to the same polynomial law for the correlations.

According to Theorem 3, we will consider a translationally invariant system with a point-symmetric Hamiltonian $(H_{QP} = H_{QP}^T)$. Following (10,11), we have to determine the entries of $(\hat{\mathcal{E}}^{-1} \oplus \hat{\mathcal{E}}^{-1})\sigma H\sigma^T$, with $\hat{\mathcal{E}} = (H_Q H_P + H_{QP}^2)^{1/2}$. In Lemma 1 we will first show that it is possible to consider the two contributions independently, and as the asymptotics of $\sigma H\sigma^T$ is known, we only have to care about the entries of $\hat{\mathcal{E}}^{-1}$, i.e., we have to determine the asymptotic behavior of the integral

$$(\hat{\mathcal{E}}^{-1})_n = \frac{1}{(2\pi)^d} \int_{\mathcal{T}^d} \mathrm{d}\phi \, \mathcal{E}^{-1}(\phi) e^{in\phi} \quad \text{where} \quad \mathcal{E} = (\hat{H}_Q \hat{H}_P + \hat{H}_{QP}^2)^{1/2}$$

Lemma 1. Given two asymptotic circulant matrices A, B in d dimensions with polynomially decaying entries, $A_n = O(||n||^{-\alpha})$, $B_n = O(||n||^{-\beta})$, $\alpha, \beta > d$. Then

$$(AB)_n = O^*(||n||^{-\mu}), \quad \mu := \min\{\alpha, \beta\}$$

Proof. With $Q_{\eta}(n) := \min\{1, ||n||^{-\eta}\}$, we know that $|A_n| = O(Q_{\alpha})$ and $|B_n| = O(Q_{\beta})$, and

$$|(AB)_n| = \left|\sum_j A_{0,j} B_{j,n}\right| \le \sum_j |A_j| |B_{n-j}| = O\left(\sum_j Q_\alpha(j) Q_\beta(n-j)\right).$$
(17)

We consider only one half space $||j|| \le ||n-j||$, where we bound $Q_{\beta}(n-j) \le Q_{\beta}(n/2)$. As $Q_{\alpha}(j)$ is summable, the contribution of this half-plane is $O(Q_{\beta}(n/2))$. The other half-plane gives the same result with α and β interchanged, which proves the bound, while tightness follows by taking all A_n , B_n positive. \Box

We now determine the asymptotics of $(\hat{\mathcal{E}}^{-1})_n$ for different types of Hamiltonians.

Lemma 2. For non-critical systems with rapidly decaying interactions, i.e., as $o(||n||^{-\infty})$, the entries of $\hat{\mathcal{E}}^{-1}$ decay rapidly as well. That is,

$$\Delta > 0 \implies (\hat{\mathcal{E}}^{-1})_n = o(\|n\|^{-\infty}).$$

Proof. As the interactions decay as $o(||n||^{-\infty})$, $\hat{H}_{\bullet} \in \mathscr{C}^{\infty}(\mathcal{T}^d)$ ($\bullet = Q, P, PQ$), and thus $\mathcal{E}^2 = \hat{H}_Q \hat{H}_P + \hat{H}_{QP}^2 \in \mathscr{C}^{\infty}(\mathcal{T}^d)$. Since the system is gapped, i.e., $\mathcal{E} \ge \Delta > 0$, it follows that also $g := \mathcal{E}^{-1} \in \mathscr{C}^{\infty}(\mathcal{T}^d)$. For the proof, we need to bound

$$(\hat{\mathcal{E}}^{-1})_n = \frac{1}{(2\pi)^d} \int_{\mathcal{T}^d} \mathrm{d}\phi \, g(\phi) e^{in\phi}$$

by $||n||^{-\kappa}$ for all $\kappa \in \mathbb{N}$. First, let us have a look at the one-dimensional case. By integration by parts, we get

$$(\hat{\mathcal{E}}^{-1})_n = \frac{1}{2\pi} \left[\frac{1}{in} g(\phi) e^{in\phi} \right]_{\phi=-\pi}^{\pi} - \frac{1}{2\pi in} \int_{-\pi}^{\pi} \mathrm{d}\phi \, g'(\phi) e^{in\phi},$$

where the first part vanishes due to the periodicity of g. As $g \in \mathscr{C}^{\infty}(\mathcal{T}^1)$, the integration by parts can be iterated arbitrarily often and all the brackets vanish, such that after κ iterations,

$$(\hat{\mathcal{E}}^{-1})_n = \frac{1}{2\pi (in)^{\kappa}} \int_{-\pi}^{\pi} \mathrm{d}\phi \, g^{(\kappa)}(\phi) e^{in\phi}.$$

As $g^{(\kappa)}(\phi)$ is continuous, the integral can be bounded by $\int |g^{(\kappa)}(\phi)| d\phi =: C_{\kappa} < \infty$, such that finally

$$|(\hat{\mathcal{E}}^{-1})_n| \leq \frac{C_{\kappa}}{n^{\kappa}} \quad \forall \kappa \in \mathbb{N} \,,$$

which completes the proof of the one-dimensional case.

The extension to higher dimensions is straightforward. For a given $n = (n_1, \ldots, n_d)$, integrate by parts with respect to the ϕ_i for which $|n_i| = ||n||_{\infty}$; we assume i = 1 without loss of generality. As $g(\cdot, \phi_2, \ldots, \phi_d) \in \mathscr{C}^{\infty}(S^1)$, the same arguments as in the 1D case show

$$|(\hat{\mathcal{E}}^{-1})_n| \leq \frac{1}{(2\pi)^d |n_1|^{\kappa}} \int_{\mathcal{T}^d} \left| \frac{\partial^{\kappa}}{\partial \phi_1^{\kappa}} g(\phi) \right| \mathrm{d}\phi = \frac{C_{\kappa}}{\|n\|_{\infty}^{\kappa}}. \quad \Box$$

For systems with *local* interactions, a stronger version of Lemma 2 can be obtained:

Lemma 3. For a system with finite range interaction, the entries of $\hat{\mathcal{E}}^{-1}$ decay exponentially.

This has been proven in [1] for Hamiltonians of the type $H = V \oplus \mathbb{1}$, exploiting a result on functions of banded matrices [26]. Following Eqs. (9,11) the generalization to arbitrary translational invariant Hamiltonians is straightforward by replacing V with $H_Q H_P - H_{QP}^2$. In fact, it has been shown recently that the result even extends to non translational invariant Hamiltonians of the form in Theorem 1 b [14].

Finally, we consider systems with polynomially decaying interaction.

Lemma 4. For a 1D lattice with $H = V \oplus 1 > 0$ and an exactly polynomially decaying *interaction*

$$V_{ij} = \begin{cases} i = j : a \\ i \neq j : \frac{b}{|i-j|^{\nu}}, & 2 \le \nu \in \mathbb{N}, \end{cases}$$

 $\hat{\mathcal{E}}^{-1}$ decays polynomially with the same exponent, $(\hat{\mathcal{E}}^{-1})_n = (V^{1/2})_n = \Theta(|n|^{-\nu}).$

Hamiltonians of this type appear, e.g., for the vibrational degrees of freedom of ions in a linear trap, where $\nu = 3$.

Proof. We need to estimate $(\hat{\mathcal{E}}^{-1})_n \stackrel{(9)}{=} (V^{-1/2})_n = \frac{1}{2\pi} \int_0^{2\pi} \hat{V}^{-1/2}(\phi) e^{in\phi} d\phi$. Note that

$$\hat{V}(\phi) = a + 2b \sum_{n=1}^{\infty} \frac{\cos(n\phi)}{n^{\nu}} = a + 2b \operatorname{Re}\left[\operatorname{Li}_{\nu}(e^{i\phi})\right] > 0,$$
(18)

where $\operatorname{Li}_{\nu}(z) = \sum_{n \ge 1} z^n / n^{\nu}$ is the polylogarithm. The polynomial decay of coefficients implies $\hat{V} \in \mathscr{C}^{\nu-2}(\mathcal{S}^1)$, and as the system is non-critical, $\hat{V}^{-1/2} \in \mathscr{C}^{\nu-2}(\mathcal{S}^1)$.

As Li_{ν} has an analytic continuation to $\mathbb{C}\setminus[1;\infty)$, $\hat{V} \in \mathscr{C}^{\infty}((0;2\pi))$ and thus $\hat{V}^{-1/2} \in \mathscr{C}^{\infty}((0;2\pi))$. We can therefore integrate by parts $\nu - 1$ times, and as all brackets vanish due to periodicity, we obtain

$$(\hat{\mathcal{E}}^{-1})_n = \frac{1}{2\pi (in)^{\nu-1}} \int_0^{2\pi} \left[\frac{\mathrm{d}^{\nu-1}}{\mathrm{d}\phi^{\nu-1}} \hat{V}^{-1/2}(\phi) \right] e^{in\phi} \mathrm{d}\phi, \tag{19}$$

and

$$\frac{\mathrm{d}^{\nu-1}}{\mathrm{d}\phi^{\nu-1}}\hat{V}^{-1/2}(\phi) = -\frac{\hat{V}^{(\nu-1)}(\phi)}{2\hat{V}(\phi)^{3/2}} + \frac{3(\nu-2)\hat{V}^{(\nu-2)}(\phi)\hat{V}^{(1)}(\phi)}{4\hat{V}(\phi)^{5/2}} + g(\phi).$$
(20)

Note that the second term only appears if $\nu \ge 3$, and g only if $\nu \ge 4$. As $g(\phi) \in \mathscr{C}^1(\mathcal{S}^1)$, its Fourier coefficients vanish as $O(n^{-1})$, as can be shown by integrating by parts. The second term can be integrated by parts as well, the bracket vanishes due to continuity, and we remain with

$$\frac{1}{in} \int_0^{2\pi} \left[\frac{3(\nu-2)\hat{V}^{(\nu-1)}(\phi)\hat{V}^{(1)}(\phi)}{4\hat{V}(\phi)^{5/2}} + h(\phi) \right] e^{in\phi} \mathrm{d}\phi,$$

with $h \in \mathscr{C}(S^1)$. [For $\nu = 3$, a factor 2 appears as $(\hat{V}^{(1)})' = \hat{V}^{(\nu-1)}$.] As we will show later, $\hat{V}^{(\nu-1)}$ is absolutely integrable, hence the integral exists, and thus the Fourier coefficients of the second term in Eq. (20) vanish as $O(n^{-1})$ as well. Finally, it remains to bound

$$\int_{0}^{2\pi} \frac{\hat{V}^{(\nu-1)}(\phi)}{2\hat{V}(\phi)^{3/2}} e^{in\phi} \mathrm{d}\phi.$$
(21)

As $\operatorname{Li}'_{\nu}(x) = \operatorname{Li}_{\nu-1}(x)/x$, it follows from Eq. (18) that

$$V^{(\nu-1)}(\phi) = 2b \operatorname{Re}\left[i^{\nu-1}\operatorname{Li}_{1}(e^{i\phi})\right] = 2b \operatorname{Re}\left[-i^{\nu-1}\log(1-e^{i\phi})\right],$$

where the last step is from the definition of Li_1 .

We now distinguish two cases. First, assume that v is even. Then,

$$V^{(\nu-1)}(\phi) \propto \text{Im}\log(1 - e^{i\phi}) = \arg(1 - e^{i\phi}) = \frac{(\phi - \pi)}{2}$$

on $(0; 2\pi)$, hence the integrand in Eq. (21) is bounded and has a bounded derivative, and by integration by parts, the integral Eq. (21) is $O(n^{-1})$. In case ν is odd we have

$$V^{(\nu-1)}(\phi) \propto \operatorname{Re}\log(1-e^{i\phi}) = \log\left|1-e^{i\phi}\right| = \log(2\sin(\phi/2))$$

on (0; 2π). With $h(\phi) := \hat{V}^{-3/2}(\phi)/2$, the integrand in Eq. (21) can be written as

$$\hat{V}^{(\nu-1)}(\phi)h(\phi) \propto \log(2\sin(\phi/2)) \ h(0) + \log(2\sin(\phi/2)) \ [h(\phi) - h(0)].$$
(22)

The first term gives a contribution proportional to

$$\int_0^{2\pi} \log(2\sin(\phi/2))\cos(n\phi)d\phi = -\frac{1}{2n}$$

as it is the back-transform of $-\frac{1}{2}\sum_{n\geq 1} \cos(n\phi)/n$. For the second term, note that $h \in \mathscr{C}^1(\mathcal{S}^1)$ for $\nu \geq 3$ and thus $h(\phi) - h(0) = h'(0)\phi + o(\phi)$ by Taylor's theorem. Therefore, the log singularity vanishes, and we can once more integrate by parts. The derivative is

$$\frac{1}{2}\cot(\phi/2) \ [h(\phi) - h(0)] + \log(2\sin(\phi/2)) \ h'(\phi).$$

In the left part, the $1/\phi$ singularity of $\cot(\phi/2)$ is cancelled out by $h(\phi) - h(0) = O(\phi)$, and the second part is integrable as $h' \in \mathcal{C}(S^1)$, so that the contribution of the integral (21) is $O(n^{-1})$ as well.

In order to show that $n^{-\nu}$ is also a lower bound on $(\hat{V}^{-1/2})_n$, one has to analyze the asymptotics more carefully. Using the Riemann-Lebesgue lemma—which says that the Fourier coefficients of absolutely integrable functions are o(1)—one finds that all terms in (19) vanish as $o(1/n^{\nu})$, except for the integral (21). Now for even ν , (21) can be integrated by parts, and while the brackets give a $\Theta(n^{-\nu})$ term, the remaining integral is $o(n^{-\nu})$, which proves that $(\hat{V}^{-1/2})_n = \Theta(n^{-\nu})$. For odd ν , on the other hand, the first part of (22) gives exactly a polynomial decay, while the contributions from the second part vanishes as $o(n^{-\nu})$, which proves $(\hat{V}^{-1/2})_n = \Theta(n^{-\nu})$ for odd ν as well. \Box

Generalizations of Lemma 4. The preceding lemma can be extended to non-integer exponents $\alpha \notin \mathbb{N}$: if $V_n \propto n^{-\alpha}$, $n \neq 0$, then $(\hat{\mathcal{E}}^{-1})_n = O(n^{-\alpha})$.

For the proof, define $\alpha = \nu + \varepsilon$, $\nu \in \mathbb{N}$, $0 < \varepsilon < 1$. Then $\hat{V} \in \mathscr{C}^{\nu-1}(\mathcal{S}^1)$, $\hat{V} \in \mathscr{C}^{\infty}((0; 2\pi))$, and one can integrate by parts ν times, where all brackets vanish. What remains is to bound the Fourier integral of the ν^{th} derivative of $\hat{V}^{-1/2}$ by $n^{-\varepsilon}$. An upper bound can be established by noting that $|\hat{V}^{(\nu)}(\phi)| \leq |\text{Li}_{\varepsilon}(e^{i\phi})| = O(\phi^{\varepsilon-1})$ and $|\hat{V}^{(\nu+1)}(\phi)| = O(\phi^{\varepsilon-2})$. It follows that all contributions in the Fourier integral except the singularity from $\hat{V}^{(\nu)}$ lead to o(1/n) contributions as can be shown by another integration by parts. In order to bound the Fourier integral of the $O(\phi^{\varepsilon-1})$ term, split the Fourier integral at $\frac{1}{n}$. The integral over $[0; \frac{1}{n}]$ can be directly bounded by $n^{-\varepsilon}$, while for $[\frac{1}{n}; 1]$, an equivalent bound can be established after integration by parts, using $\hat{V}^{(\nu+1)} = O(\phi^{\varepsilon-2})$. This method is discussed in more detail in the proof of Theorem 10, following Eq. (44).

The proof that $n^{-\varepsilon}$ is also a lower bound to $(\hat{\mathcal{E}}^{-1})_n$ is more involved. From a series expansion of \hat{V} and its derivatives, it can be seen that it suffices to bound the sine and cosine Fourier coefficients of $\phi^{\varepsilon-1}$ from below. As in the proof of Theorem 9, this is accomplished by splitting the integral into single oscillations of the sine or cosine and bounding each part by the derivative of $\phi^{\varepsilon-1}$.

For polynomially bounded interactions $V_n = O(n^{-\alpha})$, $\alpha > 1$, not very much can be said without further knowledge. With $\nu < \alpha$, $\nu \in \mathbb{N}$ the largest integer strictly smaller than α , we know that $\hat{V} \in \mathscr{C}^{\nu-1}(S^1)$. Thus, one can integrate by parts $\nu - 1$ times, the brackets vanish, and the remaining Fourier integral is o(1) using the Riemann-Lebesgue lemma. It follows that $(\hat{\mathcal{E}}^{-1})_n = o(n^{-(\nu-1)})$. In contrast to the case of an exactly polynomial decay, this can be extended to higher spatial dimensions d > 1 by replacing $\nu - 1$ with $\nu - d$, which yields $(\hat{\mathcal{E}}^{-1})_n = o(n^{-(\nu-d)})$.

We now use the preceding lemmas about the entries of $\hat{\mathcal{E}}^{-1}$ (Lemma 2–4) to derive corresponding results on the correlations of ground states of non-critical systems.

Theorem 4. For systems with $\Delta > 0$, the following holds:

(i) If the Hamiltonian H has finite range, the ground state correlations decay exponen-tially.

(ii) If H decays as o(||n||^{-∞}), the ground state correlations decay as o(||n||^{-∞}) as well.
(iii) For a 1D system with H = V ⊕ 1, where V decays with a power law |n|^{-ν}, ν ≥ 2, the ground state correlations decay as Θ(|n|^{-ν}).

Proof. In all cases, we have to find the scaling of the ground state γ which is the product $\gamma = (\hat{\mathcal{E}}^{-1} \oplus \hat{\mathcal{E}}^{-1}) \sigma H \sigma^T$, Eq. (10). Part (*i*) follows directly from Lemma 3, as multiplying with a finite-range $\sigma H \sigma^T$ doesn't change the exponential decay, while (*ii*) follows from Lemma 2, the $o(||n||^{-\infty})$ decay of $\sigma H \sigma^T$, and Lemma 1. To show (*iii*), note that for $H = V \oplus \mathbb{I}$, the ground state is $\gamma = V^{-1/2} \oplus V^{1/2}$, and from Lemma 4, $O(n^{-\nu})$ follows. For $\hat{V}^{-1/2}$, Lemma 4 also includes that the bound is exact, while for $\hat{V}^{1/2}$, it can be shown by transferring the proof of the lemma one-to-one. \Box

Note that a simple converse of Theorem 4 always holds: for each translationally invariant pure state CM γ , there exists a Hamiltonian *H* with the same asymptotic behavior as γ such that γ is the ground state of *H*. This can be trivially seen by choosing $H = \sigma \gamma \sigma^T$.

5. Correlation Length and Gap

In this section, we consider one-dimensional chains with local gapped Hamiltonians. We compute the correlation length for these systems and use this result to derive a relation between correlation length and gap.

Theorem 5. Consider a non-critical 1D chain with a local Hamiltonian. Define the complex extension of the spectral function $\mathcal{E}(\phi) = \left[\sum_{n=0}^{L} c_n \cos(n\phi)\right]^{1/2}$ in Eq. (16) as

$$g(z) := \sum_{n=0}^{L} c_n \frac{z^n + z^{-n}}{2},$$

such that $g(e^{i\phi}) = \mathcal{E}^2(\phi) \stackrel{(9)}{=} \hat{H}_Q(\phi)\hat{H}_P(\phi) - \hat{H}^2_{QP}(\phi)$ and let \tilde{z} be zero of g with the largest magnitude smaller than one. Then, the correlation length

$$\xi = -\frac{1}{\log |\tilde{z}|}$$

determines the asymptotic scaling of the correlations which is given by

- $O^*(e^{-n/\xi}/\sqrt{n})$, if \tilde{z} is a zero of order one, - $O^*(e^{-n/\xi})$, if \tilde{z} is a zero of even order, - $o(e^{-n/(\xi+\varepsilon)})$ for all $\varepsilon > 0$, if \tilde{z} is a zero of odd order larger than one.

For the nearest neighbor interaction Hamiltonian \mathcal{H}_{κ} from Eq. (1) one has for instance $\mathcal{E}(\phi) = \sqrt{1 - \kappa \cos(\phi)}$, so that g has simple zeros at $z_0 = (1 \pm \sqrt{1 - \kappa^2})/\kappa$. Therefore $\tilde{z} = (1 - \sqrt{1 - \kappa^2})/\kappa$, and the correlations decay as $\Theta(e^{-n/\xi}/\sqrt{n})$, where $\xi = -1/\log |\tilde{z}|$.

Proof. For local Hamiltonians, the correlations decay as the matrix elements of $\hat{\mathcal{E}}^{-1}$ [Eq. (10)]. By Fourier transforming (9), $\mathcal{E}(\phi) = \sqrt{g(e^{i\phi})}$, with $g(e^{i\phi}) = \hat{H}_Q(\phi)\hat{H}_P(\phi) - \hat{H}_{QP}^2(\phi) = \sum_{n=0}^{L} c_n \cos(n\phi)$ an even trigonometric polynomial (we assume $c_L \neq 0$ without loss of generality), and $\min(g(e^{i\phi})) = \Delta^2$. We have to compute

$$(\hat{\mathcal{E}}^{-1})_n = \frac{1}{2\pi} \int_0^{2\pi} \frac{1}{\mathcal{E}(\phi)} e^{in\phi} d\phi = \frac{1}{2\pi i} \int_{\mathcal{S}^1} \frac{z^{n-1}}{\sqrt{g(z)}} dz,$$
(23)

where S^1 is the unit circle. The function g(z) has a pole of order L at zero and 2L zeros altogether. Since $\min(g(\phi)) = \Delta^2 > 0$, g has no zeros on the unit circle. As g(z) = g(1/z), the zeros come in pairs, and L of them are inside the unit circle. Also, the conjugate of a zero is a zero as well. From each zero with odd multiplicity emerges a branch cut of $\sqrt{g(z)}$. We arrange all the branch cuts inside the unit circle such that they go straight to the middle where they annihilate with another cut. In case L is odd, the last cut is annihilated by the singularity of $\sqrt{g(z)}$ at 0. If two zeros lie on a line, one cut curves slightly. A sample arrangement is shown in Fig. 1.

Following Cauchy's theorem, the integral can be decomposed into integrals along the different branch cuts and around the residues of $1/\sqrt{g}$, and one has to estimate the contributions from the different types of zeros of g. The simplest case is given by zeros z_0 with even multiplicity 2m. In that case, define $h(z) := g(z)/(z-z_0)^{2m}$ which has no zero around z_0 . The contribution from z_0 to the correlations is then given by the residue at z_0 and is



Fig. 1. Sample arrangement of branch cuts and poles of \sqrt{g} inside the unit circle. From each odd order zero of g, a branch cut emerges. All cuts go to 0 where they cancel with another cut. In case their number is odd, there is an additional branch point at 0 cancelling the last cut. In case two zeros are on a line to the origin, the cuts are chosen curved. The integral of \sqrt{g} around the unit circle is equal to the integral around the cuts, plus integrals around the residues which originate from the even order zeros of g

$$\frac{1}{(m-1)!} \left. \frac{\mathrm{d}^{m-1}}{\mathrm{d}z^{m-1}} \left(\frac{z^{n-1}}{\sqrt{h(z)}} \right) \right|_{z=z_0} \propto z_0^{n-(m-1)}$$

for n - (m - 1) > 0, i.e., it scales as $|z_0|^n$. Note that for $z_0 \notin \mathbb{R}$, the imaginary parts originating from z_0 and its conjugate \overline{z}_0 exactly cancel out, but the scaling is still given by $|z_0|^n = e^{n \log |z_0|}$, i.e., $\xi = -1/\log |z_0|$ is the corresponding correlation length.

If z_0 is a simple zero of g(z), we have to integrate around the branch cut. Assume first that the cut goes to zero in a straight line, and consider a contour with distance ε to the slit. Both the contribution from the ε region around zero and the ε semicircle at z_0 vanish as $\varepsilon \to 0$, and the total integral is therefore given by twice the integral along the cut,

$$\frac{1}{\pi i}\int_0^{z_0}\frac{z^{n-1}}{\sqrt{z-z_0}\sqrt{h(z)}}\mathrm{d}z,$$

where again $h(z) = g(z)/(z - z_0)$. Intuitively, for growing *n* the part of the integral close to z_0 becomes more and more dominating, i.e., the integral is well approximated by the modified integral where h(z) has been replaced by $h(z_0)$. After rotating it onto the real axis, this integral—up to a phase—reads

$$\frac{1}{\pi\sqrt{|h(z_0)|}} \int_0^{|z_0|} \frac{r^{n-1}}{\sqrt{|z_0|-r}} \mathrm{d}r = \frac{|z_0|^{n-1/2}\Gamma(n)}{\sqrt{\pi|h(z_0)|}\Gamma(n+\frac{1}{2})},\tag{24}$$

which for large *n* is

$$\frac{1}{\sqrt{\pi |z_0 h(z_0)|}} \frac{|z_0|^n}{\sqrt{n}} + O\left(\frac{|z_0|^n}{n^{3/2}}\right).$$
(25)

In order to justify the approximation $h(z) \rightsquigarrow h(z_0)$, consider the difference of the two respective integrals. It is bounded by

$$\left| \int_{0}^{z_{0}} \frac{|z|^{n-1}}{\sqrt{|z-z_{0}|}} \underbrace{\left| \frac{1}{\sqrt{h(z)}} - \frac{1}{\sqrt{h(z_{0})}} \right|}_{(*)} dz \right|.$$

On $[z_0/2, z_0]$, h(z) is analytic and has no zeros, thus, $|h(z)^{-1/2} - h(z_0)^{-1/2}| < C|z-z_0|$, where *C* is the maximum of the derivative of $h(z)^{-1/2}$ on $[z_0/2, z_0]$. On $[0, z_0/2]$, the same bound is obtained by choosing *C* the supremum of $|h(z)^{-1/2} - h(z_0)^{-1/2}|/|z_0/2|$ on $[0, z_0/2]$. Together, $(*) \le C|z-z_0|$, and the above integral is bounded by

$$C\int_{0}^{|z_0|} r^{n-1}\sqrt{|z_0|-r} \,\mathrm{d}r = C\frac{\sqrt{\pi}|z_0|^{n+1/2}\Gamma(n)}{2\Gamma(n+\frac{3}{2})} = O\left(\frac{|z_0|^n}{n^{3/2}}\right),$$

i.e., it vanishes by 1/n faster than the asymptotics derived in Eq. (25), which justifies fixing h(z) at $h(z_0)$.

From Eq. (25), it follows that the scaling is $e^{-n/\xi}/\sqrt{n}$, where the correlation length is again $\xi = -1/\log |z_0|$. The same scaling behavior can be shown to hold for appropriately chosen curved branch cuts from z_0 to 0 by relating the curved to a straight integral.

The situation gets more complicated if zeros of odd order > 1 appear. In order to get an estimate which holds in all scenarios, we apply Cauchy's theorem to contract the unit

circle in the integration (23) to a circle of radius $r > |z_0|$, where z_0 is the largest zero inside the unit circle. Then, the integrand can be bounded by $C_r r^{n-1}$ (where $C_r < \infty$ is the supremum of $1/\sqrt{g}$ on the circle), and this gives a bound $2\pi C_r r^{n-1}$ for the integral. This holds for all $r > |z_0|$, i.e., the correlations decay faster than $e^{n \log r}$ for all $r > |z_0|$. This does not imply that the correlations decay as $e^{n \log |z_0|}$, but it is still reasonable to define $-1/\log |z_0|$ as the correlation length. \Box

Theorem 6. Consider a 1D chain together with a family of Hamiltonians $H(\Delta)$ with gap $\Delta > 0$, where $H(\Delta)$ is continuous for $\Delta \rightarrow 0$ in the sense that all entries of H converge. Then, the ground state correlations scale exponentially, and for sufficiently small Δ the correlation length is

$$\xi \simeq \frac{1}{\sqrt{\Delta m^*}}$$

Here, $m^* = \left(\frac{\mathrm{d}^2 \mathcal{E}(\phi)}{\mathrm{d}\phi^2} \Big|_{\phi = \phi_\Delta} \right)^{-1}$ *is the effective mass at the band gap.*

For the discretized Klein-Gordon field (1), for example, we have $\Delta = \sqrt{1 - |\kappa|}$, $m^* = 2\sqrt{1 - |\kappa|}/|\kappa|$, and for small Δ (corresponding to $|\kappa|$ close to 1), one obtains $\xi \simeq \sqrt{|\kappa|/2(1 - |\kappa|)} \simeq 1/\sqrt{2}\Delta$. Hence, the $\xi \propto 1/\Delta$ law holds if the coupling is increased relative to the on-site energy (in which case $m^* \propto \Delta$).

More generally, if we expand the spectral function [Eq. (16)] around the band gap we are generically³ led to the dispersion relation $\mathcal{E}(k) \simeq \sqrt{\Delta^2 + v^2 k^2}$ ($k \equiv \phi$). By the definition of the effective mass and Theorem 6 this leads exactly to the folk theorem

$$\xi \simeq \frac{v}{\Delta}.$$
(26)

Proof. According to Theorem 5, what remains to be done is to determine the position of the largest zero \tilde{z} of g in the unit circle. Due to the restriction on $H(\Delta)$, the coefficients of the polynomial $g(z)z^L$ and thus also the zeros of g continuously depend on Δ , i.e., for sufficiently small Δ , the zero closest to the unit circle is the one closest to the gap. In order to determine the position of this zero, we will expand g around the gap. We only discuss the generic case where the gap appears only for one angle $\phi_0, g(\phi_0) = \Delta$. In the case of multiple occurrences of the gap in the spectrum, one will pick the gap which gives the zero closest to the unit circle, i.e., the largest correlation length. Furthermore, we assume $\phi_0 = 0$ without loss of generality. Otherwise, one considers $g(ze^{-i\phi_0})$ instead of g(z), which on the unit circle coincides with the (rotated) spectrum.

The knowledge on g =: u + iv (with $u, v : \mathbb{C} \to \mathbb{R}$) which will be used in the proof is

$$u(1) = \Delta^{2}, \qquad v(1) = 0, u_{\phi}(1) = 0, \qquad v_{\phi}(1) = 0, u_{\phi\phi}(1) = \frac{2\Delta}{m^{*}} > 0, \qquad v_{\phi\phi}(1) = 0,$$
(27)

where the subscripts denote the partial derivative with respect to the respective subscript (in Euclidean coordinates $z \equiv x + iy$, in polar coordinates $z \equiv re^{i\phi}$). Note that

³ This makes the natural assumption that the minimum under the square root is quadratic. In fact, if it is of higher order, then $m^* = \infty$ and thus $\xi = 0$, which is consistent with the findings of the following section. An example of such a behavior is given by so called 'quadratic interactions' [2] for which $H = V \oplus \mathbb{I}$, where V is the square of a banded matrix.

z = 1 is the point where the gap appears, and that $g(e^{i\phi}) = \mathcal{E}(\phi)^2$ is real. Therefore, the derivatives of the imaginary part v along the circle vanish, while the derivatives of the real part u are found to be $u(1) = \mathcal{E}(0)^2 = \Delta^2$, $u_{\phi}(1) = 2\mathcal{E}(0)\mathcal{E}'(0) = 0$, and $u_{\phi\phi}(0) = 2\mathcal{E}'(0)^2 + 2\mathcal{E}(0)\mathcal{E}''(0) = 2\Delta/m^*$, where $m^* = 1/\mathcal{E}''(\phi)$ is the effective mass at the band gap.

We need to exploit the relation between Euclidean and polar coordinates,

$$g_x(1) = g_r(1) ; g_y(1) = g_\phi(1), g_{xx}(1) = g_{rr}(1); g_{yy}(1) = g_{\phi\phi}(1) + g_r(1),$$

and the Cauchy–Riemann equations $u_x = v_y$, $u_y = -v_x$, and $g_{xx} + g_{yy} = 0$, which together with the information (27) lead to

$$u(1) = \Delta^2; \ v(1) = 0;$$

$$u_x(1) = u_y(1) = v_x(1) = v_y(1) = 0;$$

$$u_{xx}(1) = -\frac{2\Delta}{m^*}; \ u_{yy}(1) = \frac{2\Delta}{m^*};$$

$$v_{xx}(1) = 0; \ v_{yy}(1) = 0.$$

Note that it is not possible to derive information about the mixed second derivates using only the information (27). However, as long as v_{xy} does not vanish at 1, v will only stay zero in direction of x or y, but not diagonally. Since $\Delta^2 > 0$ and $2\Delta/m^* > 0$, the closest zero is—to second order—approximately located along the x axis. By intersecting with the parabola $\Delta^2 - \frac{\Delta}{m^*}(x-1)^2$, one finds that the zero is located at $x_0 \approx 1 - \sqrt{\Delta m^*}$. For small Δ , the correlations thus decay with correlation length $\xi \approx -1/\log(1-\sqrt{\Delta m^*}) \approx 1/\sqrt{\Delta m^*}$. \Box

6. Critical Systems

In the following, we discuss critical systems, i.e., systems without an energy gap, $\Delta = 0.^4$ In that case, the Hamiltonian will get singular and some entries of the ground state covariance matrix will diverge, which leads to difficulties and ambiguities in the description of the asymptotic behavior of correlations. We will therefore restrict to Hamiltonians of the type

$$H = V \oplus \mathbb{1},$$

for which the ground state CM is $\gamma = V^{-1/2} \oplus V^{1/2}$. While the *Q* part diverges, the entries of the *P*-block stay finite. Following Thm. 1(b) the extension to interactions of the form $H = H_Q \oplus H_P$ is straightforward.

In order to compute the correlations we have to determine the asymptotics of $V^{1/2}$, i.e.,

$$(V^{1/2})_n = \frac{1}{(2\pi)^d} \int_{\mathcal{T}^d} \sqrt{\hat{V}(\phi)} e^{in\phi} \mathrm{d}\phi.$$

⁴ Note that there are different meanings of the notion criticality referring either to a vanishing energy gap or to an algebraic decay of correlations. In this section we discuss in which cases these two properties are equivalent.

We will restrict to the cases in which the excitation spectrum $\mathcal{E} = \sqrt{\hat{V}}$ has only a finite number of zeros, i.e., finitely many points of criticality. In addition, we will also consider the special case in which the Hamiltonian exhibits a tensor product structure.

We proceed as follows. First, we consider one-dimensional critical chains and show that the correlations decay typically as $O(n^{-2})$ and characterize those special cases where the correlations decay more rapidly. The practically important case of exactly cubic decaying interactions will be investigated in greater detail. Depending on the sign of the interaction this case will lead to a logarithmic deviation from the n^{-2} behavior. Then, we turn to higher dimensional systems and show that generically the correlations decay as $n^{-(d+1)} \log n$, where *d* is the spatial dimension of the lattice.

6.1. One dimension. First, we prove a lemma which shows that although taking the square root of a smooth function destroys its differentiability, the derivatives will stay bounded.

Lemma 5. Let $f \in \mathcal{C}^m([-1; 1])$, $f(x) \ge 0$ with the only zero at x = 0, and let $2\nu \le m$ be the order of the minimum at x = 0, i.e., $f^{(k)}(0) = 0 \forall k < 2\nu$, $f^{(2\nu)}(0) > 0$. Define $g(x) := \sqrt{f(x)}$. Then, the following holds:

- For odd $v, g \in \mathcal{C}^{\nu-1}([-1; 1])$, and $g \in \mathcal{C}^{m-\nu}([-1; 0])$, $g \in \mathcal{C}^{m-\nu}([0; 1])$, *i.e.*, the first m - v derivatives (for $x \neq 0$) are bounded. - For even $v, g \in \mathcal{C}^{m-\nu}([-1; 1])$.

Proof. Using the Taylor expansion $f(x) = \sum_{k=2\nu}^{m} c_k x^k + \rho(x)$, $\rho^{(k)}(x) = o(x^{m-k})$ for $k \le m$, we express g as $g(x) = (\operatorname{sgn} x)^{\nu} x^{\nu} r(x)$ with

$$r(x) = \sqrt{\sum_{k=2\nu}^{m} c_k x^{k-2\nu} + \frac{\rho(x)}{x^{2\nu}}},$$

where we used that $(\operatorname{sgn} x)^{\nu} x^{\nu} = \sqrt{x^{2\nu}}$. Let us now consider the derivatives of r(x). While the sum leads to a O(1) contribution, the k^{th} derivative of the remainder behaves as $o(1)/x^{2\nu-m+k}$. Together, this leads to

$$r^{(k)}(x) = O(1), \qquad 2\nu - m + k \le 0,$$

$$r^{(k)}(x) = o(1)/x^{2\nu - m + k}, \qquad 2\nu - m + k \ge 1.$$

Now consider the k^{th} derivative of g(x) for $x \neq 0$,

$$g^{(k)}(x) = (\operatorname{sgn} x)^{\nu} \sum_{l=0}^{k} \underbrace{\binom{k}{l} \left[\frac{\mathrm{d}^{l}}{\mathrm{d}x^{l}} x^{\nu} \right] r^{(k-l)}(x)}_{s_{l}}.$$

Assume first $k \leq v$. Then, $s_l \propto O(1)x^{\nu-l}$ for $2\nu - m + k - l \leq 0$, and $s_l \propto O(1)x^{m-\nu-k}$ for $2\nu - m + k - l \geq 1$, and as $m \geq 2\nu$, it follows that $g^{(k)} = O(x)$ for $k < \nu$, which cancels the discontinuity originating from sgn x. For $k = \nu$, on the contrary, $s_k = O(1)$, and sgn x introduces a discontinuity on $g^{(k)}$, yet, it remains bounded and piecewise differentiable on [-1; 0] and [0; 1]. The first non-bounded s_l is found as soon as $m - \nu - k = -1$, and $g \in \mathcal{C}^{m-\nu}([0; 1])$ directly follows.

This also implies that for $m - \nu - k \ge 0$, $g(x)/(\operatorname{sgn} x)^{\nu} \in \mathcal{C}^{m-\nu}([-1; 1])$, i.e., the discontinuity is only due to $(\operatorname{sgn} x)^{\nu}$. Since, however, this is only discontinuous for odd ν , it follows that $g \in \mathcal{C}^{m-\nu}([-1; 1])$ if ν even. \Box

Theorem 7. Consider a one-dimensional critical chain with Hamiltonian $H = V \oplus \mathbb{1}$, where $V_n = O(n^{-\alpha})$, $\alpha > 4$ and where \hat{V} has a finite number of critical points which are all quadratic minima of \hat{V} . Then, $(\gamma_P)_n = O^*(n^{-2})$. For $V_n \propto n^{-\alpha}$, $\alpha > 3$ it even follows that $(\gamma_P) = \Theta(n^{-2})$.

Note that for $V_n \propto n^{-\alpha}$, the extrema of \hat{V} are always quadratic.

Proof. We want to estimate

$$(V^{1/2})_n = \frac{1}{2\pi} \int_{\mathcal{S}^1} g(\phi) e^{in\phi} \mathrm{d}\phi,$$
 (28)

where $g = \hat{V}^{1/2}$. Under both assumptions, $\hat{V} \in \mathscr{C}^2(\mathcal{S}^1)$, and all critical points are minima of order 2. It follows from Lemma 5 that g is continuous with bounded derivative. Therefore, we can integrate by parts, the bracket vanishes, and we obtain

$$(V^{1/2})_n = -\frac{1}{2\pi i n} \int_0^{2\pi} g'(\phi) e^{in\phi} \mathrm{d}\phi$$

Now, split S^1 at the zeros of g into closed intervals \mathcal{I}_j , $\bigcup_j \mathcal{I}_j = S^1$, and rewrite the above integral as a sum of integrals over \mathcal{I}_j . As $g' \in \mathscr{C}(\mathcal{I}_j)$ (and differentiable on the inner of \mathcal{I}_j), one can once more integrate by parts which yields

$$(V^{1/2})_n = -\frac{1}{2\pi (in)^2} \sum_j \left(\left[g'(\phi) e^{in\phi} \right]_{\mathcal{I}_j} - \int_{\mathcal{I}_j} g''(\phi) e^{in\phi} d\phi \right).$$
(29)

Neither of the terms will vanish, but since $g' \in \mathcal{C}(\mathcal{I}_j)$, the bracket is bounded. In case $V_n \in O(n^{-\alpha}), \alpha > 4$, we have $\hat{V} \in \mathcal{C}^3(S^1)$, therefore g'' is bounded (Lemma 5), and the integrals vanish as o(1). Unless the contributions of the brackets for the different \mathcal{I}_j cancel out, the n^{-2} bound is tight, $(V^{1/2})_n = O^*(n^{-2})$. The tightness of the bound is also illustrated by the example which follows the proof.

For the case of an exactly polynomial decay, we additionally have to show that g'' is absolutely integrable for $3 < \alpha \le 4$. Then, the exactness of the bound holds because the bracket in Eq. (29) does not oscillate (the critical point is either at $\phi = 0$ or at $\phi = \pi$), and because the integral is o(1) for $g'' \in \mathcal{L}^1(\mathcal{S}^1)$. In case the critical point is at $\phi = \pi$, the latter holds since $\hat{V} \in \mathscr{C}^{\infty}((0; 2\pi))$ implies that g'' is bounded at π , and $\hat{V} \in \mathscr{C}^2(\mathcal{S}^1)$ that $g \in \mathscr{C}^2((-\pi, \pi))$, which together proves that g'' is bounded on \mathcal{S}^1 .

In case the critical point is at $\phi = 0$, the situation is more involved (and for $\alpha = 3$, a logarithmic correction appears, cf. Theorem 9). Since $\hat{V}^{(3)}(\phi) = -\text{Im}[\text{Li}_{\alpha-3}(e^{i\phi})] = O(\phi^{\alpha-4})$, we have

$$\begin{split} \hat{V}''(\phi) &= \hat{V}''(0) + O(\phi^{\alpha-3}), \\ \hat{V}'(\phi) &= \hat{V}''(0)\phi + O(\phi^{\alpha-2}), \\ \hat{V}(\phi) &= \frac{1}{2}\hat{V}''(0)\phi^2 + O(\phi^{\alpha-1}). \end{split}$$

With this information,

$$g''(\phi) = \frac{2\hat{V}(\phi)\hat{V}''(\phi) - \hat{V}'(\phi)^2}{4V(\phi)^{3/2}} = O(\phi^{\alpha-4}),$$

which indeed proves that $g'' \in \mathcal{L}^1(\mathcal{S}^1)$, and thus $(V^{1/2})_n = \Theta(n^{-2})$. \Box

As an example, consider again the discretized Klein-Gordon field of Eq. (1) which is critical for $\kappa = \pm 1$, corresponding to $\hat{V}(\phi) = 1 \mp \cos \phi$. The Fourier integral is solvable and yields $(\gamma_P)_n = -\frac{2\sqrt{2}}{\pi} \frac{(\operatorname{sgn} \kappa)^n}{4n^2 - 1} = \Theta(n^{-2})$.

Generalizations of Theorem 7. Using Lemma 5, several generalizations for the 1D critical case can be found. In the following, we mention some of them. In all cases $H = V \oplus \mathbb{1}$ is critical.

Critical points of even order. If $V_n = o(n^{-\infty})$ and the critical points are minima of order 2ν , ν even, the correlations decay as $(\gamma_P)_n = o(n^{-\infty})$. This is the case, e.g., if $V = X^2$ with X itself rapidly decaying.

Critical points of higher order. If \hat{V} has critical points of order at least 2ν , ν odd, and $V_n = O(n^{-\alpha})$, $\alpha > 2\nu + 2$, then $(\gamma_P)_n = O(n^{-(\nu+1)})$.

Minima of different orders. If \hat{V} has minima of different orders $2\nu_i$, in general the minimum with the lowest odd $\nu_i \equiv \nu_1$ will determine the asymptotics, $(\gamma_P)_n = O(n^{-(\nu_1+1)})$. As $\hat{V} \in \mathscr{C}^{(2\max\{\nu_i\})}(S^1)$ is required anyway, the piecewise differentiability of $\hat{V}^{1/2}$ is guaranteed.

Weaker requirements on V. It is possible to ease the requirements imposed on V in Theorem 7 to $V_n = O(n^{-\alpha}), \alpha > 3$ or $\hat{V} \in \mathscr{C}^2(S^1)$, respectively. The price one has to pay is that one gets an additional log correction as in the multidimensional critical case, Theorem 10. The method to bound g'' is the same which is used there to derive (39).

The above proof does not cover the case of the relevant $1/n^3$ interaction, which for instance appears for the motional degrees of freedom of trapped ions. In the following, we separately discuss this case. It will turn out that the scaling will depend on the sign of the coupling: while a positive sign (corresponding to the radial degrees of freedom) again gives a $\Theta(\frac{1}{n^2})$ scaling as before, for the negative sign (corresponding to the axial degree of freedom) one gets $\Theta(\frac{\sqrt{\log n}}{n^2})$.

Theorem 8. Consider a critical 1D chain with a $1/n^3$ coupling with positive sign, i.e., $H = V \oplus \mathbb{1}$, $V_n = c/n^3$, $V_0 = 3c\zeta(3)/2$, c > 0, with ζ the Riemann zeta function. Then, the ground state correlations scale as $(\gamma_P)_n = \Theta(\frac{1}{n^2})$.

Proof. We take w.l.o.g. c = 1/2. For this sign of the coupling, the critical point is at π , $\hat{V}(\pi) = 0$. From the proof of Lemma 4, we know that $\hat{V} \in \mathscr{C}^1(\mathcal{S}^1)$, $\hat{V} \in \mathscr{C}^{\infty}((0; 2\pi))$, and that $\hat{V}''(\phi) = \log(2\sin(\phi/2))$ on $(0; 2\pi)$. With $g := \hat{V}^{1/2}$, it follows from Lemma 5 that $g \in \mathscr{C}(\mathcal{S}^1)$, $g \in \mathscr{C}^1([-\pi; \pi])$, and $g \in \mathscr{C}^{\infty}((0; \pi])$, $g \in \mathscr{C}^{\infty}([-\pi; 0])$. This means that all derivatives $g^{(k)}$, $k \ge 1$ can exhibit jumps at the critical point π but they all remain bounded. In contrast, around $\phi = 0$, g' is continuous but g'' has a log divergence.

Thus, the Fourier integral

$$(V^{1/2})_n = \frac{1}{2\pi} \int_{\mathcal{S}^1} g(\phi) e^{in\phi} \mathrm{d}\phi$$

can be split at 0 and π , and then integrated by parts twice. The brackets of the first integration cancel out due to continuity of *g*, and one remains with

$$(V^{1/2})_n = \frac{1}{\pi (in)^2} \left(\left[g'(\phi) \cos(n\phi) \right]_0^{\pi} + \int_0^{\pi} g''(\phi) \cos(n\phi) d\phi \right),$$

where we used the symmetry of g. One finds $[g'(\phi) \cos(n\phi)]_0^{\pi} = -\sqrt{\frac{\log 2}{2}}(-1)^n$, and since g'' is integrable, the integral is o(1) due to the Riemann-Lebesgue lemma. Together, this proves $(\gamma_P)_n = \Theta(\frac{1}{n^2})$. \Box

Theorem 9. Consider a critical 1D chain with a $1/n^3$ coupling with negative sign, i.e., $H = V \oplus \mathbb{1}$, $V_n = -c/n^3$, $V_0 = 2c\zeta(3)$, c > 0, with ζ the Riemann zeta function. Then, the ground state correlations scale as $(\gamma_P)_n = \Theta(\frac{\sqrt{\log n}}{n^2})$.

Proof. Again, take w.l.o.g. c = 1/2. For the negative sign of the interaction, the critical point is at $\phi = 0$. Since at this point \hat{V}'' diverges, Lemma 5 cannot be applied, and the situation gets more involved.

As in the previous proof, we use that $\hat{V} \in \mathscr{C}^1(\mathcal{S}^1)$, $\hat{V} \in \mathscr{C}^{\infty}((0; 2\pi))$, and thus $\hat{V}^{1/2} \in \mathscr{C}(\mathcal{S}^1)$, $\hat{V}^{1/2} \in \mathscr{C}^{\infty}((0; 2\pi))$. Further, $\hat{V}''(\phi) = -\log(2\sin(\phi/2))$ on $(0; 2\pi)$, cf. the proof of Lemma 4, and with $\sin x = x(1 + O(x^2))$ we have $\hat{V}''(\phi) = -\log(\phi) + O(\phi^2)$ for $\phi \to 0$ (and similarly for $\phi \to 2\pi$), and therefore

$$\hat{V}'(\phi) = \phi(1 - \log \phi) + O(\phi^3), \quad \hat{V}(\phi) = \frac{1}{4}\phi^2(3 - 2\log \phi) + O(\phi^4).$$
 (30)

As $\hat{V}^{1/2} \in \mathscr{C}(\mathcal{S}^1)$, we can integrate by parts one time,

$$(V^{1/2})_n = \frac{1}{2\pi} \int_{\mathcal{S}^1} \hat{V}^{1/2}(\phi) e^{in\phi} d\phi = \frac{1}{\pi n} \int_0^\pi g'(\phi) \sin(n\phi) d\phi,$$
(31)

where we exploited the symmetry of \hat{V} , and with $g := \hat{V}^{1/2}$. Then, from (30),

$$g'(\phi) = \frac{1 - \log \phi}{\sqrt{3 - 2\log \phi}} + O\left(\frac{\phi^2}{\sqrt{|\log \phi|}}\right), \ g''(\phi) = \frac{-2 + \log \phi}{\phi (3 - 2\log \phi)^{3/2}} + O\left(\frac{\phi}{\sqrt{|\log \phi|}}\right),$$

and after another round of approximation,

$$g'(\phi) = \frac{\sqrt{|\log \phi|}}{\sqrt{2}} + O\left(\frac{1}{\sqrt{|\log \phi|}}\right), \ g''(\phi) = -\frac{1}{2^{3/2}} \frac{1}{\phi\sqrt{|\log \phi|}} + O\left(\frac{1}{\phi|\log \phi|^{3/2}}\right).$$

This shows that the remainder $g'(\phi) - \sqrt{|\log \phi|/2|}$ is continuous with an absolutely integrable derivative, and by integration by parts it follows that it only leads to a contribution O(1/n) in the integral (31). Thus, it remains to investigate the asymptotics of the sine Fourier coefficients of $h(\phi) = \sqrt{|\log \phi|}$. For convenience, we split the integral (31) at 1, and $[1; \pi]$ only contributes with O(1/n), as *h* is continuous with absolutely integrable derivative on $[1; \pi]$. On [0; 1], we have to compute the asymptotics of

$$\mathcal{I} = \int_0^1 \sqrt{-\log\phi} \sin(n\phi) \mathrm{d}\phi.$$
(32)

Therefore, split the integral at 1/n. The left integral can be bounded directly, and the right after integration by parts [cf. the treatment of Eq. (44)]. One gets

$$\mathcal{I} \leq \int_0^{1/n} \sqrt{-\log\phi} \, \mathrm{d}\phi + \frac{\sqrt{\log n}}{n} + \frac{1}{n} \int_{1/n}^1 \frac{1}{2\phi\sqrt{-\log\phi}} \mathrm{d}\phi = O\left(\frac{\sqrt{\log n}}{n}\right).$$

In order to prove that this is also a lower bound for the asymptotics, it suffices to show this for the integral (32) as all other contributions vanish more quickly. To this end, split

the integral (32) into single oscillations of the sine, $J_k = \left[\frac{2\pi k}{n}, \frac{2\pi (k+1)}{n}\right], k \ge 0$. As $\sqrt{-\log \phi}$ has negative slope on (0; 1), each of the J_k gives a positive contribution to \mathcal{I} , and thus we can truncate the integral at $\frac{1}{2}$,

$$\mathcal{I} \ge \sum_{\frac{2\pi(k+1)}{n} \le \frac{1}{2}} \int_{J_k} \sqrt{-\log \phi} \, \sin(n\phi) \, \mathrm{d}\phi.$$
(33)

On $[0; \frac{1}{2}]$, $\sqrt{-\log \phi}$ has a positive curvature, and thus, each of the integrals can be estimated by linearly approximating $\sqrt{-\log \phi}$ at the middle of each J_k but with the slope at $\frac{2\pi(k+1)}{n}$, which gives

$$\int_{J_k} \sqrt{-\log \phi} \, \sin(n\phi) \, \mathrm{d}\phi \ge \frac{\pi}{n^2} \frac{1}{\frac{2\pi(k+1)}{n} \sqrt{-\log\left[\frac{2\pi(k+1)}{n}\right]}}$$

Now, we plug this into the sum (33) and bound the sum by the integral from $\frac{2\pi}{n}$ to $\frac{1}{2}$ (the integrand in monotonically decreasing), which indeed gives a lower bound $\frac{1}{n}(\sqrt{\log \frac{n}{2\pi}} - \sqrt{\log 2})$ on \mathcal{I} and thus proves the $\Theta(\sqrt{\log n}/n^2)$ scaling. \Box

6.2. Higher dimensions. For more than one dimension, the situation is more involved. First of all, it is clear by taking many uncoupled copies of the one-dimensional chain that there exist cases where the correlations will decay as n^{-2} . However, these are very special examples corresponding to Hamiltonians with a tensor product structure $H_{i_1i_2,j_1j_2} = H_{i_1,j_1}H'_{i_2,j_2}$. In contrast, we show that for generic systems the correlations in the critical case decay as $O(n^{-(d+1)} \log n)$, where *d* is the dimension of the lattice. The requirement is again that the energy spectrum $\mathcal{E}(\phi)$ has only a finite number of zeroes, i.e., finitely many critical points.

Note that the case of a Hamiltonian with a tensor product structure can also be solved, as in that case \hat{V} becomes a product of terms depending on one ϕ_i each and thus the integral factorizes. Interestingly, although the correlations along the axes decay as n^{-2} , the correlations in a fixed diagonal direction will decay as $n_1^{-2} \cdots n_d^{-2} \propto ||n||^{-2d}$ and thus even faster than in the following theorem. The $O(||n||^{-(d+1)} \log ||n||)$ decay of the theorem holds isotropically, i.e., independent of the direction of n.

Theorem 10. Consider a *d*-dimensional bosonic lattice with a critical Hamiltonian $H = V \oplus \mathbb{1}$. Then the *P*-correlations of the ground state decay as

$$O\left(\|n\|^{-(d+1)}\log\|n\|\right)$$

if the following holds: $\hat{V} \in \mathcal{C}^{d+1}$ [e.g., the correlations decay as $O(||n||^{-(2d+1+\varepsilon)})$, $\varepsilon > 0$], \hat{V} has only a finite number of zeros which are quadratic minima, i.e., the Hessian $\left(\frac{\partial^2 \hat{V}(\phi)}{\partial \phi_i \partial \phi_j}\right)_{ii}$ is positive definite at all zeros.

Proof. We have to evaluate the asymptotic behavior of the integral

$$(\hat{V}^{1/2})_n = \frac{1}{(2\pi)^d} \int_{\mathcal{T}^d} \mathrm{d}^d \phi \sqrt{\hat{V}(\phi)} \cos[n\phi].$$

Let us first briefly sketch the proof. We start by showing that it suffices to analyze each critical point separately. To this end, we show that is is possible to smoothly cut out some environment of each critical point which reproduces the asymptotic behavior. Then, we rotate the coordinate system such that we always look at the correlations in a fixed direction, and integrate by parts—which surprisingly can be carried out as often as \hat{V} is differentiable, as all the brackets vanish. Therefore, the information about the asymptotics is contained in the remaining integral, and after a properly chosen number of partial integrations, we will attempt to estimate this term.

Let now ζ_i , i = 1, ..., I be the zeros of \hat{V} . Clearly, these will be the only points which contribute to the asymptotics as everywhere else $\sqrt{\hat{V}}$ is \mathscr{C}^{d+1} . In order to separate the contributions coming from the different ζ_i , we will make use of so-called *neutralizers* [27]. For our purposes, these are functions $\mathcal{N}_{\xi_0,r} \in \mathscr{C}^{\infty}(\mathbb{R}^d \to [0; 1])$ which satify

$$\mathcal{N}_{\xi_0, r}(\xi) = \begin{cases} 1 : \|\xi - \xi_0\| \le r/2\\ 0 : \|\xi - \xi_0\| \ge r \end{cases}$$

and are rotationally symmetric (cf. [27] for an explicit construction). For each ζ_i , there exists an r_i such that the balls $B_{r_i}(\zeta_i)$ do not intersect. We now define the functions

$$f_i(\phi) := \sqrt{\hat{V}(\phi)} \mathcal{N}_{\zeta_i, r_i}(\phi), \quad \rho(\phi) := \sqrt{\hat{V}(\phi)} - \sum_{i=1}^I f_i(\phi).$$

Clearly, ρ is \mathscr{C}^{d+1} , and so is each f_i except at ζ_i . Furthermore, each f_i is still the square root of a \mathscr{C}^{d+1} function. By definition,

$$(\hat{V}^{-1/2})_n = \frac{1}{(2\pi)^d} \sum_{i=1}^I \int_{\mathcal{T}^d} \mathrm{d}^d \phi f_i(\phi) \cos[n\phi] + \frac{1}{(2\pi)^d} \int_{\mathcal{T}^d} \mathrm{d}^d \phi \rho(\phi) \cos[n\phi], \quad (34)$$

i.e., it suffices to look at the asymptotics of each f_i separately. The contribution of ρ is $O(||n||^{-(d+1)})$ as can be shown by successive integrations by parts just as for the non-critial lattice (cf. the proof of Lemma 2).

Let us now analyze the integrals

$$I_i = \int_{B_{r_i}(\zeta_i)} \mathrm{d}^d \phi f_i(\phi) \cos[n\phi].$$

The integration range can be restriced to $B_{r_i}(\zeta_i)$ as f_i vanishes outside the ball. By a rotation, this can be mapped to an integral where n = (||n||, 0, ..., 0), whereas f_i is rotated to another function \tilde{f}_i with the same properties,

$$I_i = \int_{B_{r_i}(\zeta_i)} \mathrm{d}^d \phi \, \tilde{f}_i(\phi) \cos[\|n\|\phi_1].$$

Since the integrand is continuous and thus bounded, it is absolutely integrable, and from Fubini's theorem, one finds

$$I_{i} = \int_{B_{r_{i}}(\tilde{\zeta}_{i})} \mathrm{d}^{d-1}\tilde{\phi} \underbrace{\int_{\zeta_{i,1}-r_{i}}^{\zeta_{i,1}+r_{i}} \mathrm{d}\phi_{1}\tilde{f}_{i}(\phi_{1},\tilde{\phi})\cos[\|n\|\phi_{1}]}_{J_{i}(\tilde{\phi})},$$

where we separated out the integration over the first component. The vector $\tilde{\phi}$ denotes the components 2...d of ϕ . The extension of the integration range to a cylinder is possible as \tilde{f}_i vanishes outside $B_{r_i}(\zeta_i)$.

Let us now require $\tilde{\phi} \neq \tilde{\zeta}_i$. This does not change the integral since the excluded set is of measure zero, but it ensures that \tilde{f}_i is in \mathcal{C}^{d+1} . This allows us to integrate the inner integral $J_i(\tilde{\phi})$ by parts up to d + 1 times, and each of the brackets

$$\left[\tilde{f}_{i}^{(k)}(\phi_{1},\tilde{\phi})\frac{1}{\|n\|^{k}}\cos(\|n\|\phi_{1}-k\pi/2)\right]_{\phi_{1}=\zeta_{i,1}-r_{i}}^{\zeta_{i,1}+r_{i}}$$

appearing in the k^{th} integration step vanishes. Here, $\tilde{f}_i^{(d)}(\phi_1, \tilde{\phi}) = \partial^d \tilde{f}_i(\phi_1, \tilde{\phi})/\partial \phi_1^d$ is the d^{th} partial derivative with respect to the first argument. After integrating by parts d times, we obtain

$$I_{i} = \frac{1}{\|n\|^{d}} \int d^{d-1} \tilde{\phi} \int d\phi_{1} \tilde{f}_{i}^{(d)}(\phi_{1}, \tilde{\phi}) \cos[\|n\|\phi_{1} - d\pi/2].$$
(35)
$$B_{r_{i}}(\tilde{\zeta}_{i}) \qquad \zeta_{i,1} - r_{i}$$

Now we proceed as follows: first, we show that the order of integration can be interchanged, and second, we show that for the function obtained after integrating $\tilde{f}_i^{(d)}$ over $\tilde{\phi}$, the Fourier coefficients vanish as $\log(||n||)/||n||$.

The central issue for what follows is to find suitable bounds on $|\tilde{f}_i^{(k)}|$. Therefore, define $\tilde{f}_i^2 =: h_i \in \mathcal{C}^{d+1}$. By virtue of Taylor's theorem, and as $h_i(\zeta_i) = 0$ is a minimum,

$$h_i(\phi) = \frac{1}{2}(\phi - \zeta_i) \cdot (\mathbf{D}^2 h_i(\zeta_i))(\phi - \zeta_i) + o(\|\phi - \zeta_i\|^2)$$

with \mathbf{D}^2 the second derivative. As the first term is bounded by $\frac{1}{2} \|\mathbf{D}^2 h_i(\zeta_i)\|_{\infty} \|\phi - \zeta_i\|^2$ and the second vanished faster than $\|\phi - \zeta_i\|^2$, we can find $\varepsilon_i > 0$ and $C_1 > 0$ such that

$$|h_i(\phi)| \le C_1 \|\phi - \zeta_i\|^2 \quad \forall \|\phi - \zeta_i\| < \varepsilon_i.$$
(36)

By looking at the Tayor series of $h'_i \equiv \partial h_i / \partial \phi_1$ up to the first order we also find that there are $\varepsilon_i > 0$ and $C_2 > 0$ such that

$$|h_i'(\phi)| \le C_2 \|\phi - \zeta_i\| \qquad \forall \|\phi - \zeta_i\| < \varepsilon_i.$$
(37)

In addition to these upper bounds, we will also need a lower bound on $|h_i|$. Again, by the Taylor expansion of h_i around ζ_i , we find

$$|h_i(\phi)| \ge \lambda_{\min} \left[\mathbf{D}^2 h_i(\zeta_i) \right] - o(\|\phi - \zeta_i\|^2),$$

and as all the zeros are quadratic minima, i.e., $\lambda_{\min} \left[\mathbf{D}^2 h_i(\zeta_i) \right] > 0$, there exist $\varepsilon_i > 0$, $C_3 > 0$ such that

$$|h_i(\phi)| \ge C_3 \|\phi - \zeta_i\|^2 \qquad \forall \|\phi - \zeta_i\| < \varepsilon_i.$$
(38)

Clearly, ε_i can be chosen equal in Eqs. (36–38). Note that the bounds can be chosen to be invariant under rotation of h_i and thus of \tilde{f}_i . This holds in particular for the ε_i as the remainders of Taylor series vanish uniformly. Thus, the bound we will obtain for the correlation function indeed only depends on ||n|| and not on the direction of n.

Now, we use the conditions (36–38) to derive bounds on $|\tilde{f}_i^{(k)}|$. Therefore, note that from $\tilde{f}_i \equiv \sqrt{h_i}$ it follows that

$$\tilde{f}_{i}^{(k)} = \frac{\sum_{\substack{j_{1}+\dots+j_{k}=k\\j_{\nu}=0,1,2,\dots}} c_{j_{1}\dots j_{k}} h_{i}^{(j_{1})} \cdots h_{i}^{(j_{k})}}{h_{i}^{(2k-1)/2}}.$$

One can easily check that for each term in the numerator, the number K_0 of zeroth derivatives and the number K_1 of first derivatives of h_i satisfy $2K_0 + K_1 \ge k$. By bounding all higher derivatives of h_i from above by constants, we find that the modulus of each summand in the numerator, and thus the modulus of the numerator itself, can be bounded above by $C' \| \phi - \zeta_i \|^k$ in the ball $B_{\varepsilon_i}(\zeta_i)$ with some C' > 0. On the other hand, it follows directly from (38) that the modulus of the denominator is bounded below by $C'' \| \phi - \zeta_i \|^{2k-1}$, C'' > 0, such that in total

$$|\tilde{f}_i^{(k)}(\phi)| \le C \frac{1}{\|\phi - \zeta_i\|^{k-1}}; \quad 1 \le k \le d+1.$$
(39)

Note that this holds not only inside $B_{\varepsilon_i}(\zeta_i)$ but in the whole domain of f_i , as outside $B_{\varepsilon_i}(\zeta_i)$, f_i is \mathscr{C}^{d+1} and thus all the derivatives are bounded. Equation (39) is the key result for the remaining part of the proof. First, it can be

Equation (39) is the key result for the remaining part of the proof. First, it can be used to bound the integrand in (35) by an integrable singularity (this is most easily seen in spherical coordinates, where $1/r^{d-1}$ is integrable in a *d*-dimensional space). Hence, the order of integration in (35) can be interchanged, and it remains to investigate the asymptotics of the integral

$$I_{i} = \frac{1}{\|n\|^{d}} \int_{\zeta_{i,1} - r_{i}}^{\zeta_{i,1} + r_{i}} d\phi_{1}g_{i}(\phi_{1})\cos[\|n\|\phi_{1} - d\pi/2], \text{ with }$$
(40)

$$g_i(\phi_1) \equiv \int_{B_{r_i}(\tilde{\zeta}_i)} \mathrm{d}^{d-1}\tilde{\phi} \ \tilde{f}_i^{(d)}(\phi_1, \tilde{\phi}). \tag{41}$$

From (39), we now derive bounds on $g_i(\phi_1)$ and its first derivative. Again, we may safely fix $\phi_1 \neq \zeta_{i,1}$ as this has measure zero. Then, using (39) we find that

$$|g_i(\phi_1)| \le \int_0^{r_i} \frac{C}{\left((\phi_1 - \zeta_{i,1})^2 + r^2\right)^{(d-1)/2}} S_{d-1} r^{d-2} \mathrm{d}r,$$

where we have transformed into spherical coordinates $[S_{d-1}]$ is the surface of the (d-1)-dimensional unit sphere] and assumed the l_2 -norm. Since $(\phi_1 - \zeta_1)^2 + r^2 \ge r^2$, the integrand can be bounded once again, and we find

$$|g_{i}(\phi_{1})| \leq \int_{0}^{r_{i}} \frac{CS_{d-1}}{((\phi_{1} - \zeta_{i,1})^{2} + r^{2})^{1/2}} dr$$

= $C\left(-\log|\phi_{1} - \zeta_{i,1}| + \log\left[r_{i} + \sqrt{r_{i}^{2} + (\phi_{1} - \zeta_{i,1})^{2}}\right]\right)$
 $\leq -C\log|\phi_{1} - \zeta_{i,1}|,$ (42)

where in the last step we used that in (40) $|\phi_1 - \zeta_{i,1}| < r_i$ and that r_i can be chosen sufficiently small.

Next, we derive a bound on $g'_i(\phi_1)$. As we fix $\phi_1 \neq \zeta_1$, the integrand in (41) is \mathscr{C}^1 and we can take the differentiation into the integral,

$$g'_i(\phi_1) = \int_{B_{r_i}(\tilde{\xi}_i)} \mathrm{d}^{d-1}\tilde{\phi}\tilde{f}_i^{(d+1)}(\phi_1,\tilde{\phi}).$$

Again, we bound the integrand by virtue of Eq. (39) and obtain

$$|g_{i}'(\phi_{1})| \leq \int_{0}^{r_{i}} \frac{CS_{d-1}}{((\phi_{1} - \zeta_{i,1})^{2} + r^{2})} dr$$

= $C \frac{\arctan\left[\frac{r_{i}}{|\phi_{1} - \zeta_{i,1}|}\right]}{|\phi_{1} - \zeta_{i,1}|} \leq \frac{C'}{|\phi_{1} - \zeta_{i,1}|}.$ (43)

Finally, these two bounds will allow us to estimate (40) and thus the asymptotics of the correlations in the lattice. We consider one half of the integral (40),

$$\int_{\zeta_{i,1}}^{\zeta_{i,1}+r_i} d\phi_1 g_i(\phi_1) \cos[\|n\|\phi_1 - d\pi/2],$$
(44)

as both halves contribute equally to the asymptotics. We then split the integral at $\zeta_{i,1} + r_i / ||n||$. The left part gives

$$\begin{vmatrix} \zeta_{i,1}+r_i/\|n\| \\ \int \\ \zeta_{i,1} \\ d\phi_1 g_i(\phi_1) \cos[\|n\|\phi_1 - d\pi/2] \\ \leq \int \\ \zeta_{i,1} \\ \zeta_{i,1} \\ d\phi_1(-\log|\phi_1 - \zeta_{i,1}|) \\ = \frac{r_i - r_i \log r_i + r_i \log\|n\|}{\|n\|}.$$
(45)

The right part of the split integral (44) can be estimated by integration by parts,

$$\begin{vmatrix} \zeta_{i,1}+r_{i} \\ \int \\ \zeta_{i,1}+r_{i}/\|n\| \\ \leq \left| \left[g_{i}(\phi_{1}) \frac{1}{\|n\|} \cos[\|n\|\phi_{1}-(d+1)\pi/2] \right]_{\zeta_{i,1}+r_{i}/\|n\|}^{\zeta_{i,1}+r_{i}} \right| + \frac{1}{\|n\|} \int_{\zeta_{i,1}+r_{i}/\|n\|}^{\zeta_{i,1}+r_{i}} d\phi_{1}|g_{i}'(\phi_{1})| \\ \stackrel{(42,43)}{\leq} C \frac{\log\|n\|}{\|n\|} + C' \frac{|\log r_{i}|}{\|n\|}.$$

$$(46)$$

Thus, both halves [Eqs. (45),(46)] give a $\log ||n||/||n||$ bound for the integral (44), and thus the integral I_i is asymptotically bounded by $\log ||n||/||n||^{d+1}$ following Eq. (40). As the number of such integrals in (34) is finite, this proves that the correlations of the ground state decay at least as $\log ||n||/||n||^{d+1}$. \Box

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