Entanglement Spectra of Spin Chains

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Abstract We discuss the use of entanglement spectra in analysing spin chains. First discovered in the context of many-body ground states in fractional quantum Hall effect, entanglement spectra facilitate the resolution of the phenomenology of a spin chain. In particular, this includes its nature of low-energy excitations and topological classification.

1 Entanglement Spectra of Many-Body Ground States

Quantum entanglement encodes the essence of quantum mechanical phenomenology. It allows to describe aspects of interconnectivity of quantum systems which go beyond the notion of correlations and sets the basis for potential future technological applications of quantum systems for communication, information processing and computation. Entanglement also helps a great deal to analyse and classify quantum systems. This particularly applies to the entanglement entropy, which has appeared as a useful tool in a broad and diverse range of theoretical physics [4, 17]. By comparison, the computation of entanglement spectra is a rather new approach added to the theorist's toolkit to analyse quantum many-body systems, which was initiated in the context of fractional quantum Hall effect [14]. There, an important observation was made for the entanglement analysis of a fractional quantum Hall ground state with an excitation gap on a spherical geometry [8]. The entanglement spectrum resulting from a decomposition of the Hilbert space into an upper and lower hemisphere allowed to read off the state counting and quantum numbers of elementary edge excitations the same quantum Hall state would exhibit on a disc geometry, which thus gives way to resolving the topological order of a given ground state wave function. The analysis of entanglement spectra has ever since become an indispensable approach to analyse wave functions in different many-body contexts,

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including spin chains. Among other pioneering findings resulting from there, it is the perspective of entanglement spectra which has allowed for a fairly complete understanding of interacting topological phases in one spatial dimension [21].

The purpose of this chapter is to introduce the reader to the principal topic, through discussing a selection of key ideas that have proven pivotal to our today's understanding of entanglement spectra in spin chains. This synopsis does neither intend to be complete nor self-contained but hopes to encourage the reader to deepen their understanding by following up on it via the additional literature within and beyond the chapter. The chapter is organised as follows. In Sect. 2, we provide a principal definition of entanglement spectra for the context in which we intend to discuss it. This means that we highlight those Hilbert space decompositions, and their descendant entanglement spectra, which so far have been considered in the context of spin chains. In order to present the material in a concise way, it proves useful to classify spin chains by the existence or absence of an excitation gap. Section 3 focusses on entanglement spectra for gapped spin chains, which is explicated by a discussion of the Haldane phase from multiple perspectives. Section 4 discusses entanglement spectra for gapless spin chains at the example of the spin-1/2 Heisenberg chain. In Sect. 5, we conclude that entanglement spectra will continue to establish a vital tool for future research on spin chains.

It is assumed that the reader will be triggered by many interesting connections to other chapters in this book. In order to avoid overlap, we intend to sharply constrain ourselves to the topic of entanglement spectra, with only occasional highlighting of connections drawn to other subfields of quantum spin chains.

2 Decomposition of Spin Chain Hilbert Spaces

In the following, we assume a zero-temperature density operator ρ, which is determined by a spin chain ground state $|\Psi_0\rangle$, i.e., $\rho = |\Psi_0\rangle\langle\Psi_0|$. Assuming a tensor product decomposition of the spin chain Hilbert space into a region A and B according to $\mathscr{H} = \mathscr{H}_A \times \mathscr{H}_B$, we define the reduced density matrix

$$\rho_A := \mathrm{Tr}_B \rho. \tag{1}$$

Since Tr_B represents a partial trace, ρ_A is not invariant under a unitary transformation of $|\Psi_0\rangle$ in $\mathscr{H}$. Stated differently, ρ_A is basis-dependent and hence crucially depends on how $\mathscr{H}$ is decomposed. Assuming a Schmidt decomposition according to

$$|\Psi_0\rangle = \sum_\alpha \lambda_\alpha \, |\alpha A\rangle \, |\alpha B\rangle \,, \tag{2}$$

the eigenvalues of ρ_A are λ_α^2. Following a form-invariant Boltzmann-type definition according to ρ, we define an entanglement Hamiltonian

$$\rho_A =: \exp(-H_\mathrm{E}), \tag{3}$$

where the temperature scale is set to unity. The entanglement spectrum $\{\xi_\alpha\}$ is defined as the spectrum of H_E, which relates to the spectrum of ρ_A, and hence the Schmidt decomposition (2), via $\xi_\alpha = -2\log\lambda_\alpha$.

Since the early days of quantum entanglement, these quantities have been known and appear in any definition of quantum information measures such as the entanglement entropy $S_A = -\mathrm{Tr}\rho_A\log\rho_A$, which will likely be extensively covered in other chapters of this book. Furthermore, properties of the entanglement spectrum for non-interacting problems have likewise been studied previously [18]. The key insight put forward in [14] in the context of quantum many-body physics is to analyse the block diagonal structure or, equivalently, the symmetries of ρ_A. Obviously, this depends on the chosen cut as much as on $|\Psi_0\rangle$. If a real space cut is chosen and $|\Psi_0\rangle$ is a spin singlet, we find $[S_A^\gamma, \rho_A] = 0$, where $S_A^\gamma = \sum_{i\in A} S_i^\gamma$, $\gamma = x, y, z$, which yields an SU(2) multiplet structure $[\mathbf{S}_A^2, \rho_A] = 0$, characterised by the eigenvalues $s_A(s_A+1)$. For a finite-size spin chain and periodic boundary conditions (Fig. 1a up), the decomposition of a compact state always yields two bonds subject to the subdivision into regions A and B. (Note that this will constrain s_A to SO(3) multiplets.) For a non-compact semi-infinite real space cut (Fig. 1a down), the decomposition reduces to a single bond. In general, all those symmetries of $|\Psi_0\rangle$ are projectively inherited by ρ_A that allow for a symmetry operator decomposition which is commensurate with the chosen cut. For the rung cut of a spin ladder (Fig. 1b), for instance, all symmetries are accordingly retained that concern one individual chain of the ladder. In particular, if we assume a spin ladder ground state

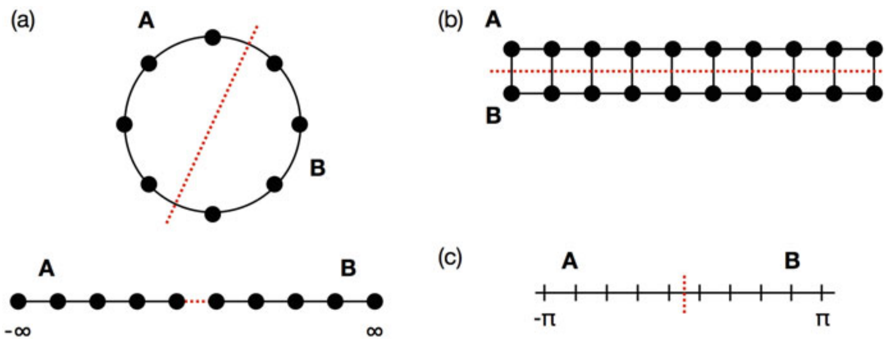

Fig. 1 Typical entanglement cuts for spin chains. (**a**) Real space cut. For finite-size and periodic boundary conditions, the partition into subregions yields two cuts (marked dashed red). In a quasi-infinite real space representation such as for matrix product states, a single cut is performed. (**b**) Rung cut. A spin ladder ribbon is divided into subregions of individual chains. (**c**) Momentum cut. All momentum modes are split into two different subregions of momenta

for periodic boundary conditions, this includes translation symmetry along the spin chain. For any momentum cut (Fig. 1c) of a spin chain, the details of which will be described later, a representation of $|\Psi_0\rangle$ is required in terms of momentum modes, which are then grouped into different regions A and B.

There are in principle several other entanglement cuts which have been used in the context of many-body ground states and which might acquire scientific relevance for spin chains in the future. Among others, this includes the particle cut [26], where a reduced density matrix is reached by integrating out particle modes while leaving the single particle Hilbert space unspoiled. Such a particle cut would promise a particular use in combination with the momentum cut.

3 Gapped Spin Chains

For a spin chain spectrum with an energy gap, $\rho = |\Psi_0\rangle\langle\Psi_0|$ is rigorously defined in the thermodynamic limit. Furthermore, due to locality and the exponential decay of correlation functions due to the gap, a real space cut suggests itself as a natural choice.

In order to elucidate the power of an entanglement spectrum analysis of gapped spin chains, we choose the Haldane phase as a textbook example to illustrate the concepts. The Haldane phase [7, 9] found its first realisation in SU(2) symmetric spin-1 chains and is a symmetry protected topological phase in one spatial dimension [24]. Before a rigorous entanglement spectral analysis had been formulated, the necessary and sufficient symmetry conditions for the Haldane phase had not been completely resolved. The issue had been that while certain topological classifications such as through a non-local string order parameter [13] proved to be the correct indicator in the presence of certain other supporting symmetries, the parametric realisation range of the Haldane phase exceeded the one of the string order. Similarly, the Haldane phase seemed to transcend the regime in which a ground state realisation of the Haldane phase for open boundary conditions would show degenerate edge states in line with the bulk-boundary correspondence of topological phases.

We start by employing a Haldane phase ground state realisation from the bilinear-biquadratic (bb) SU(2) spin-1 Hamiltonian class $H_{\text{bb}} = \sum_i \cos\theta \mathbf{S}_i\mathbf{S}_{i+1} + \sin\theta(\mathbf{S}_i\mathbf{S}_{i+1})^2$, where the Haldane phase is found for $-\pi/4 \leq \theta \leq \pi/4$. As shown in Fig. 2a and explained above, the entanglement spectrum reveals an SO(3) multiplet structure according to s_A [30]. The dominant entanglement weight is carried by a singlet and a triplet state, while the rest of the entanglement levels appear to be separated by a gap. Note that for the AKLT point [1], the triplet and singlet level would be the only non-zero weights λ, i.e., the only finite entanglement spectral eigenvalues.

If we were to diagonalise H_{bb} on an open chain, we would obtain a similar low-energy spectrum. By analogy to the lessons from entanglement spectra for fractional quantum Hall effect, this observation provokes the hypothesis that the entanglement

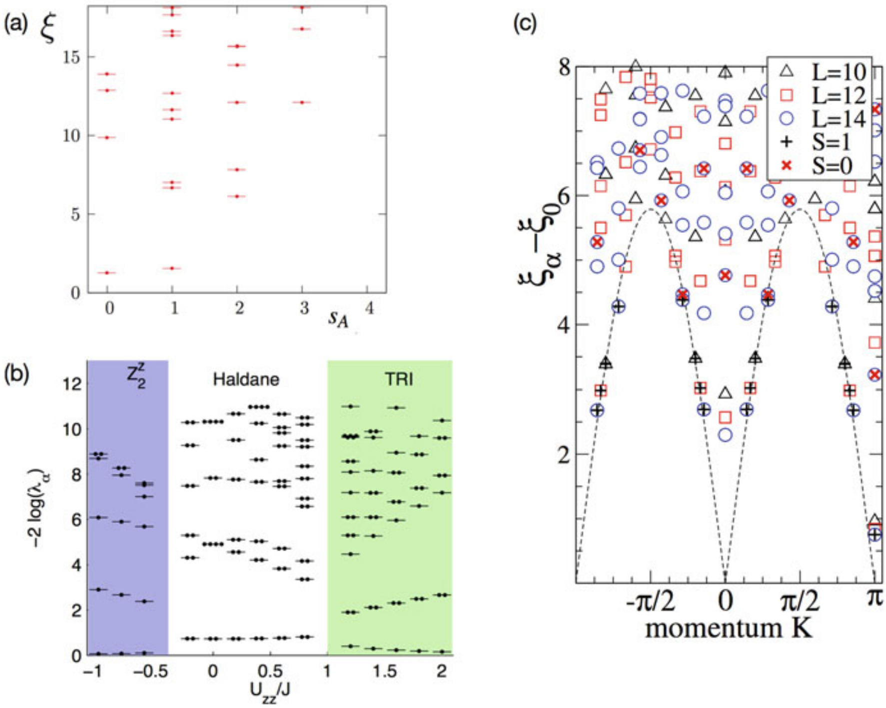

Fig. 2 Entanglement cuts in the Haldane phase. (**a**) Finite-size real space cut for an $N = 12$ site ground state of H_{bb} against the multiplet index s_A [30]. (**b**) Semi-infinite real space cut of H_{ju} as a function of U_{zz}/J [21]. (**c**) Rung cut for a ground state of H_{sl} plotted against the chain momentum and offset by the lowest entanglement level ξ_0 [20]

spectrum of a spin-1 chain ground state for periodic boundary conditions relates to the low-energy spectrum of the same Hamiltonian for open boundaries [23]. More careful finite-size scaling shows that this is indeed true. For a topological phase with dimensionally reduced edge mode excitations, it is suggestive that such a real space entanglement cut induces entanglement eigenstates of dominant weight λ (and hence the lowest value ξ) which feature related properties to energy edge modes of the open chain.

Further information beyond the compact real space cut can be retrieved from a semi-infinite real space cut [21]. This is conveniently obtained through a matrix product state (MPS) representation of $|\Psi_0\rangle$:

$$|\Psi_0\rangle = \lim_{N\to\infty} \sum_{\{m\}} \mathrm{Tr}\Gamma_{m_1}\Lambda\Gamma_{m_2}\Lambda\ldots\Gamma_{m_N}\Lambda\,|m_1 m_2 \ldots m_N\rangle\,, \tag{4}$$

where m_i denotes the $S_i^z = -1, 0, 1$ eigenvalue for a spin-1 chain. A gapped spin chain allows for a finite matrix representation of Γ_{m_i} and Λ, where the eigenvalues of Λ are the λ_α's in (2). Furthermore, in anticipation of resolving the Haldane phase according to its core topological structure free from overlaying superfluous symmetries, we investigate the MPS ground state representation of the Hamiltonian $H_{\mathrm{ju}} = \sum_i J\mathbf{S}_i\mathbf{S}_{i+1} + U_{\mathrm{zz}}(S_i^z)^2$. Here, starting from the spin-1 Heisenberg chain, the U_{zz} term breaks the SU(2) symmetry. (A complete symmetry analysis with additional terms is discussed in [21, 22]). By monitoring the eigenvalues of Γ, the semi-infinite real space cut (Fig. 1a down) is realised. The core insight of [21] is that the entanglement spectrum provides us with a necessary and sufficient criterion for the Haldane phase: as visible in Fig. 2b, the Haldane phase is characterised by an even multiplicity of Schmidt eigenvalues for the entire entanglement spectrum. This roots in the fact that the irreducible projective symmetry representations in the Haldane phase must be higher dimensional, which accordingly brings about the spectral degeneracy. As a side remark, one readily observes that departing from $U_{zz}/J = 0$, the breaking of SU(2) symmetry shows no spectral relevance for the Haldane phase. It is already suggestive from here that the successful entanglement spectrum classification of the Haldane phase generalises to other gapped topological phases in one dimension [31].

Spin chain spectra can also emerge as the entanglement Hamiltonian of spin ladders [20]. We investigate a spin-1/2 ladder ribbon given by the Hamiltonian $H_{\mathrm{sl}} = \sum_i J_\parallel(\mathbf{S}_i^I\mathbf{S}_{i+1}^I + \mathbf{S}_i^{II}\mathbf{S}_{i+1}^{II}) + J_\perp\mathbf{S}_i^I\mathbf{S}_i^{II}$, where $J_\parallel$ ($J_\perp$) denotes the coupling along the chains (between the chains I and II). For $J_\parallel > 0$ and $J_\perp < 0$, this yields another realisation of the Haldane phase. Performing a rung cut according to Fig. 1c, along with spin rotation symmetry, the reduced density matrix keeps translation symmetry along the chain, which allows the resolution of the entanglement spectrum with respect to chain momentum (Fig. 2c). Both in terms of spectral and eigenstate structure, the entanglement Hamiltonian resulting from the rung cut of the ground state of H_{sl} is similar to the energy spectrum of a spin-1/2 Heisenberg spin chain.

4 Gapless Spin Chains

Our assumed hitherto definition of ρ as a projector onto a spin chain ground state appears particularly reasonable for the case of a gapped spin chain in the zero-temperature limit. It is less transparent how to go about a gapless spin chain, where ρ should be susceptible to arbitrarily weak perturbations. The hallmark results from entanglement entropy for real space cuts, however, suggest a different perspective [2]. The entanglement entropy exhibits a scaling law $S_A \propto (c/3)\log l$, where l is the length of the real space interval A and c is the central charge of the associated conformal field theory. Due to this result, the entanglement entropy has become one of the paradigmatic parameters to retrieve from the finite-size realisation of a given spin chain Hamiltonian, which is particularly amenable to numerical observability [5, 19]. While no strong spectral resemblance is expected between the energy spectrum and the associated entanglement spectrum as we encountered for gapped spin chains, a lesson from real space cuts of gapless spin chains is that fundamental features of the physical systems can still be extracted from the entanglement spectrum and its derivative quantities.

An extended momentum cut (Fig. 1c) performed on the ground state of a gapless spin chain Hamiltonian helps to resolve a universal fingerprint of its critical theory [16, 27]. To illustrate this hypothesis, we consider spin-1/2 spin chains on even-membered rings with periodic boundary conditions. The N sites are placed on a circle of radius unity and are thus described by the Nth roots of unity: $z_j = \exp(2\pi i j/N)$; $j \in \{1, \ldots, N\}$. Any singlet ground state of an SU(2)-invariant Hamiltonian in hardcore boson notation takes the form

$$|\Psi_0\rangle = \sum_{j_1,\ldots,j_K} \psi(z_{j_1}, \ldots, z_{j_K}) S^-_{j_1} \ldots S^-_{j_K} |F\rangle , \tag{5}$$

where $|F\rangle = |\uparrow \ldots \uparrow\rangle$ is a polarised reference state. The sum extends over all ways to distribute $K = \frac{1}{2}N$ down-spins on the ring, and the weights $\psi(z_{j_1}, \ldots, z_{j_K})$ depend only on the position of the spin $\downarrow$ sites. We Fourier transform the spin operators on each site according to $\tilde{S}^-_m = \frac{1}{N}\sum_j z_j^m S^-_j$ so that

$$|\Psi_0\rangle = \sum_{m_1,\ldots,m_K} \tilde{\psi}(m_1, \ldots, m_K) \tilde{S}^-_{m_1} \ldots \tilde{S}^-_{m_K} |F\rangle , \tag{6}$$

where

$$\tilde{\psi}(m_1, \ldots, m_K) = N^{-K} \sum_{j_1,\ldots,j_K} z_{j_1}^{m_1} \ldots z_{j_K}^{m_K} \psi(z_{j_1}, \ldots, z_{j_K}). \tag{7}$$

This extended momentum monomial basis is non-orthogonal and represented by bosonic occupation numbers n_m for crystal momentum m, yielding a total state momentum $M = \sum_m m n_m$. The total particle number is given by $K = \sum_m n_m$ and the physical crystal momentum by $Q = M \bmod N$. The regions A and B for the extended momentum cut are decomposed with respect to the number of particles and total momentum according to $N_A + N_B = N$ and $M_A + M_B = M$. The extended momentum hence bears close resemblance to the entanglement cut on a quantum Hall sphere, where the momentum M_A is replaced by the angular momentum on the hemisphere L_A [14]. The entanglement spectrum for a spin-1/2 Heisenberg chain is plotted in Fig. 3.

To better understand the relation between the extended momentum cut entanglement spectra and the critical theory of a gapless spin chain, it is best to start from the viewpoint of the Haldane–Shastry (HS) model [10, 25], a spin-1/2 chain which, due to its Yangian quantum group structure [11], resolves the Wess–Zumino–Witten (WZW) SU(2)$_1$ field theory at finite size without logarithmic corrections. Furthermore, the HS ground state wave function, aside from a gauge factor to ensure

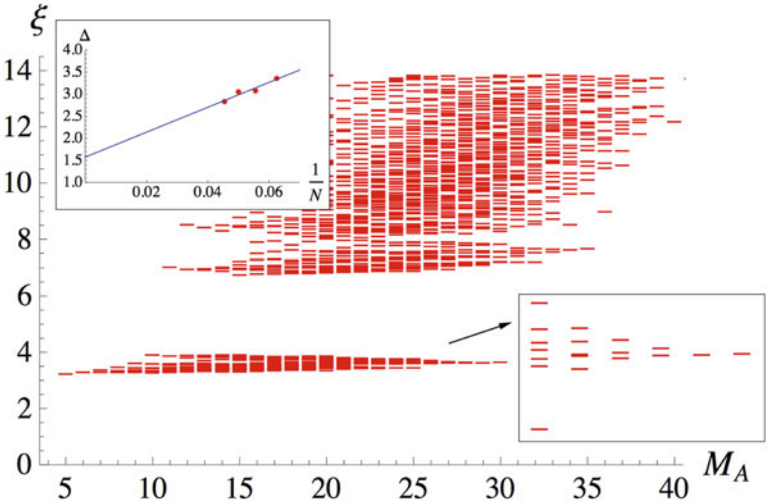

Fig. 3 Extended momentum entanglement cut for the spin-1/2 Heisenberg spin chain [27]. A low entanglement energy manifold is separated from higher level contributions through an entanglement gap Δ which persists in the thermodynamic limit (left inset). The state counting of the low-lying levels matches that of a bosonic U(1) state counting (right inset)

its singlet property, matches the form of the bosonic Laughlin fractional quantum Hall state at magnetic filling $\nu = 1/2$:

$$\psi_{\mathrm{HS}} = \prod_{i<j}^{K} (z_i - z_j)^2 \prod_{i=1}^{K} z_i. \tag{8}$$

One finds that the entanglement spectrum of the HS ground state is composed of only few eigenstates of ρ_A with finite entanglement weight and a large remainder part with zero entanglement weight, i.e., $\xi \to \infty$. Furthermore, the state count per sector M_A reads $1, 1, 2, 3, 5, 7, \ldots$ and thus agrees with the $U(1)$ bosonic state counting which matches the low-energy excitations of this universality class of gapless spin chains. (Note that such state countings are subtle and necessitate a significant system size for unambiguous resolution. This is because, for instance, a counting $1, 1, 2, 3, 5, 8, \ldots$ would have hinted at a Fibonacci state counting.) The upshot of the extended momentum cut is that for the entire spin-1/2 fluid phase including the Heisenberg spin chain, which is described by $\mathrm{SU}(2)_1$ WZW field theory, these levels serve as the low entanglement Hamiltonian spectral fingerprint. Figure 3 depicts the extended momentum cut entanglement spectrum for the spin-1/2 Heisenberg chain. The low-energy part is the universal component, which in terms of state counting and eigenstates is identical to the HS point. All other entanglement levels are higher up in entanglement energy and separated by an entanglement gap Δ which appears to persist in the thermodynamic limit. While the $U(1)$ state counting can only conveniently be resolved through the extended momentum cut with respect to M, the entanglement gap would still be visible for a crystal momentum cut with respect to Q. This entanglement gap frames a notion of topological adiabaticity, where two spin chain models are defined to be topologically connected if the entanglement gap from their ground state momentum cut persists along the interpolation [28]. To which extent this hypothesis is applicable to arbitrary gapless models in one spatial dimension, or in fact the predictive power of entanglement spectra in general still is a subject of debate [3, 15].

The extended momentum cut appears suitable to resolve deconfined spinon excitations of gapless spin chains. The HS model, which can be thought of as the free spinon gas related to SU(2)$_1$ WZW field theory where the spinons only interact through their fractional statistics, plays a similar role for the extended momentum cut entanglement spectra as the AKLT point does for the real space cut entanglement spectra of the Haldane phase. Subsequent studies of gapless spin chains with other critical theories such as the SU(2)$_2$ and SU(3)$_1$ WZW field theory [16] suggest that the extended momentum cut indeed serves as a way to resolve the low-energy critical theory of spin chains from the entanglement analysis of finite-size ground state wave functions. Here, the analogue to the HS Point for SU(2)$_k$ WZW field theories is formed by the Greiter $S = k/2$ spin chain Hamiltonians [6, 29].

5 Conclusion

The strong dependence of entanglement spectra on the chosen cut inhibits advantages and drawbacks at the same time. We could witness the former in this chapter, where the right cut adjusted to the spin chain at hand would allow one to learn in tremendous detail about the spin chain properties solely from the ground state wave function. Regarding the latter, it is still a matter of ongoing research to determine under which conditions there is reliable universality extractable from entanglement spectra [3, 15]. Furthermore, due to its manifest basis-dependent, i.e., gauge-dependent character, it is a subtle question whether any of these entanglement spectra immediately relate to observable quantities. As one promising sign in this direction, the measurement of entanglement entropy has at least been successfully performed in a highly tunable and accessible environment of ultra-cold gases deposited into an optical lattice [12], while the knowledge of all Renyi entropies would in principle allow to reconstruct the entanglement spectrum.

Despite these open questions, it is evident that entanglement spectra have become an indispensable diagnosis tool for quantum many-body systems in general and spin chains in particular. It should be considered likely that further fundamental insights will be gained from future entanglement spectral analyses of spin chains.

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