Entropic analysis of quantum phase transitions from uniform to spatially inhomogeneous phases

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We propose a new approach to study quantum phase transitions in low-dimensional fermionic or spin models that go from uniform to spatially inhomogeneous phases such as dimerized, trimerized, or incommensurate phases. It is based on studying the length dependence of the von Neumann entropy and its corresponding Fourier spectrum for finite segments in the ground state of finite chains. Peaks at a nonzero wave vector are indicators of oscillatory behavior in decaying correlation functions.

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Recently, it has been shown [1] that, quite generally, discontinuities in some measure of entanglement between different parts of a ground-state quantum system can be used to study quantum phase transitions (QPTs). This measure can be the concurrence [2], which can be used to study spin-1/2 models [3, 4, 5, 6, 7, 8, 9], the entropy of a block of length sites [13], or, more generally, the entropy of a block of length [13, 14].

In a parallel development, it has been pointed out that critical and noncritical systems behave differently [15, 16] when the length dependence of the entropy of a finite segment of a quantum system is studied. The von Neumann entropy of a subsystem of length \( l \) (measured here and subsequently in units of the lattice constant \( a \)) saturates at a finite value when the system is noncritical, i.e., when the spectrum is gapped, while it increases logarithmically for critical, gapless systems. An analytic expression has been derived for models that map to a conformal field theory [17], and this form has been shown to be satisfied by critical spin models. The entropy for a subsystem of length \( l \) in a finite system of length \( N \) has been shown to be [18]

\[
s(l) = \frac{c}{6} \ln \left( \frac{2N}{\pi} \sin \left( \frac{\pi l}{N} \right) \right) + g, \tag{1}
\]

where \( c \) is the central charge and \( g \) is a constant shift due to the open boundary which depends on the ground-state degeneracy [13].

The aim of this paper is to show that the length dependence of the von Neumann entropy of a subsystem can, in fact, display a much richer structure than discussed until now, and that its analysis allows a better characterization of the QPT, thereby providing a new diagnostic tool to study QPTs. Moreover, this method seems to be appropriate to study cases when no true phase transition takes place, i.e., when only the character of the decaying correlation function changes. Our method is especially convenient when the density-matrix renormalization-group (DMRG) algorithm [20] is used, in which the density matrix of blocks of different lengths are generated in the course of the procedure so that the von Neumann entropy can be easily calculated.

The first, simplest case which we will consider is the Majumdar-Ghosh (MG) model [21], which corresponds to the frustrated spin-1/2 Heisenberg chain, described by the Hamiltonian

\[
\mathcal{H} = \sum_i \left[ J(S_i \cdot S_{i+1}) + J'(S_i \cdot S_{i+2}) \right], \tag{2}
\]

at the particular parameter value \( J' = 0.5J \). Since the ground state (of a finite chain) consists of independent nearest-neighbor singlets between odd and even sites, the entropy of a segment of length \( l \) oscillates between \( \ln 2 \) when the block has an unpaired spin at its end and 0 when all spins in the block are paired into singlets [21]. We will also consider the exactly solvable Takhtajan-Babujian (TB) [22] and Uimin-Lai-Sutherland (ULS) [23] points of the spin-one bilinear-biquadratic model [24],

\[
\mathcal{H} = \sum_i \left[ \cos \theta (S_i \cdot S_{i+1}) + \sin \theta (S_i \cdot S_{i+1})^2 \right], \tag{3}
\]

which correspond to the parameter values \( \theta = -\pi/4 \) and \( \pi/4 \), respectively. As shown in Fig. 1 a periodic oscillation is superimposed onto a curve that is described by the analytic form given by Eq. (1) in both cases. At the TB point, the period of oscillation is two lattice sites, while at the ULS point it is three lattice sites. When the length \( l \) is taken to be a multiple of two for the TB point or a multiple of three for the ULS, the entropy \( s(l) \) can be well-fitted using Eq. (1) with \( c \) approaching the known values, \( c = 3/2 \) [25] and \( c = 2 \) [26], respectively, in the limit of large \( N \).

In order to analyze the oscillatory nature of the finite subsystem entropy \( s(l) \), it is useful to consider its Fourier
FIG. 1: Length dependence of the von Neumann entropy of segments of length \( l \) of a finite chain with \( N = 60 \) sites for (a) the Takhtajan-Babujian and (b) the Uimin-Lai-Sutherland models. The solid lines are our fit using Eq. (1) taking every second and third data points.

The spectrum

\[ \tilde{s}(q) = \frac{1}{N} \sum_{l=0}^{N} e^{-iql}s(l), \]

with \( s(0) = s(N) = 0 \) where \( q = 2\pi n/N \) and \( n = -N/2, \ldots, N/2 \). Since \( s(l) \) satisfies the relation \( s(l) = s(N-l) \), its Fourier components are all real and symmetric. \( \tilde{s}(q) = \tilde{s}(-q) \); therefore, only the \( 0 \leq q \leq \pi \) region will be shown. Except for the large positive \( \tilde{s}(q = 0) \) component that grows with increasing chain length, the other components are all negative. They are shown for the two cases discussed above in Fig. 2. As can be seen, apart from the \( q = 0 \) point, the Fourier spectrum exhibits negative peaks at \( q = \pi \) and \( q = 2\pi/3 \), respectively. This is related to the fact that the TB model has two soft modes, at \( q = 0 \) and \( \pi \), while the ULS model has three, at \( q = 0 \) and \( \pm 2\pi/3 \). Although finite-size extrapolation shows that these components vanish in the \( N \rightarrow \infty \) limit, these peaks in the Fourier spectrum are nevertheless indications that the decay of correlation functions is not simply algebraic in these critical models, but that the decaying function is multiplied by an oscillatory factor. When the same calculation is performed for \( \theta \) in the range \(-3\pi/4 < \theta < -\pi/4 \), where the system is gapped and dimerized, the peak at \( q = \pi \) remains finite as \( N \rightarrow \infty \).

We demonstrate this procedure on the example of the spin-one bilinear-biquadratic model near the VBS point [27], corresponding to \( \theta_{\text{VBS}} = \arctan \frac{1}{3} \sim 0.1024\pi \). It is known [28] that this point is a disorder point, where incommensurate oscillations appear in the decaying correlation function; however, the shift of the minimum of the static structure factor appears only at a larger \( \theta_{1} = 0.138\pi \), the so-called Lifshitz point. In earlier work [13], some of us showed that \( s(N/2) \) has an extremum as a function of \( \theta \) at \( \theta_{\text{VBS}} \). Here we show that this extremum is the indication that, in fact, \( \theta_{\text{VBS}} \) is a dividing point which separates regions with a different behavior of \( s(l) \) and \( \tilde{s}(q) \).

As usual in the DMRG approach, we consider open chains. The numerical calculations were performed using the dynamic block-state selection (DBSS) approach [29]. The threshold value of the quantum information loss \( \chi \) was set to \( 10^{-8} \) for the spin models and to \( 10^{-4} \) for the fermionic model, and the upper cutoff on the number of block state was set to \( M_{\text{max}} = 1500 \).

At and below the VBS point, i.e., for \(-\pi/4 < \theta \leq \theta_{\text{VBS}} \), \( s(l) \) increases with \( l \) for small \( l \), saturates due to the Haldane gap [30], and then goes down to zero again as \( l \) approaches \( N \). The Fourier spectrum \( \tilde{s}(q) \) is a smooth function of \( q \) (except for the \( q = 0 \) component). The transformed entropy \( \tilde{s}(q) \) at the VBS point, depicted in Fig. 3 illustrates this behavior. For \( \theta \) slightly larger than \( \theta_{\text{VBS}} \), however, we find that \( s(l) \) does not increase to the saturation value purely monotonically. Instead, an incommensurate oscillation is superimposed. For somewhat larger \( \theta \) values, \( \theta > 0.13\pi \), this oscillation persists in the saturated region, i.e., for blocks much longer than the correlation length. This leads to a new peak in \( \tilde{s}(q) \) which moves from small \( q \) towards \( q = 2\pi/3 \) as the ULS point is approached, and gets larger and narrower, as can
be seen in Fig. 3. This $\theta$ value is slightly smaller than, but close to, the Lifshitz point.

The spin-1/2 frustrated Heisenberg chain, Hamiltonian (2), is also known to develop incommensurate correlations, for values of $J'/J > 0.5$ (the MG point). As shown in Fig. 4, the entropies of blocks of length $N/2$ and $N/2 + 1$, although substantially different in value, both display a minimum as a function of $J'/J$ at the MG point. Thus, the transition from commensurate (dimerized) to incommensurate correlations again is marked by an extremum of the block entropy. Similarly to the behavior in the neighborhood of the VBS point, in this model a long wavelength oscillation appears in $s(l)$ right above $J'/J > 0.5$, which leads to a new peak in the Fourier spectrum. The displacement with increasing $J'/J$ is in this case, however, towards $q = \pi/2$, as can be seen in Fig. 5. This peak becomes larger and narrower for increasing $J'/J$, and again is a signature of incommensurability.

It is also interesting to examine the behavior of the block entropy in the lowest-lying triplet excited states. This is shown in Fourier-transformed representation, $\tilde{s}(q)$, in Fig. 6 for several $J'/J$ values. At $J' = 0.5J$, the peak at $q = \pi$ is displaced to $q = \pi(1 - 1/N)$. As $J'/J$ increases, we find two oppositely moving peaks. One appears exactly where the peak was found for the ground state, while the other occurs at $\pi - q$. By also calculating the structure factor, $S(q)$, we found that this second peak is located at the same ($J'/J$-dependent) wave vector at which $S(Q)$ has its maximum $\tilde{s}$. For Hamiltonian (3), the block entropy of the first triplet state also has two oppositely moving peaks. One is again at the same location as the incommensurate peak in the ground state, while the other is at $\pi - q/2$. Both peaks move towards $2\pi/3$ with increasing $\theta$.

Having demonstrated the usefulness of studying the entropy profiles for models where the quantum critical points are known, we now use this procedure to study an commensurate-incommensurate transition in the 1D $t - t' - U$ Hubbard model

$$\mathcal{H} = t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma}) + t' \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+2\sigma} + c_{i+2\sigma}^\dagger c_{i,\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (5)$$

which has been investigated recently $\bar{3}$. For the half-
filled case (and setting $t = 1$), the competition between $t'$ and the Coulomb energy $U$ will determine whether the system is an insulator ($t' < t''_c$) or a metal ($t' > t''_c$). For finite $U$ values, the transition between these two states occurs in two steps. First the spin gap opens at $t''_s$ and then the charge gap closes at a larger value $t''_t$. Between these two points, the wave vector becomes incommensurate for $t' > t''_c$ – the commensurate-incommensurate transition is independent of the metal-insulator transition.

As expected for a commensurate-incommensurate transition, we find that the entropy of blocks of length $N/2$ and $N/2 + 1$ display an extremum as a function of $t'$. For very large $U$ values, where the model is equivalent to the frustrated spin-$1/2$ Heisenberg chain, the extremum occurs at $t''_c \approx 1/\sqrt{2}$, which maps to the MG point. For $t' > t''_c$, an incommensurate oscillation in $s(l)$ becomes apparent. This behavior can be seen in Fig. 7 for $U = 3$, a value chosen so that our results can be directly compared to those of Ref. [32]. When $s(q)$ is analyzed, it is found that a new peak appears in the spectrum and again moves from small $q$ towards $q = \pi/2$ with the amplitude of $s(q)$ decreasing with increasing $t'$. Therefore, the commensurate-incommensurate phase boundary can be easily determined by finding the extrema of $s(N/2)$ as a function of $t'$ for various $U$ values. The detailed entropy analysis of the full two-dimensional phase diagram will be presented in subsequent work.

In conclusion, we have shown that the length dependence of the block entropy and its Fourier spectrum, determined for finite systems, can be used to characterize phases in which the correlation function has an oscillatory character. In addition, an extremum in the block entropy as a function of the relevant model parameter, which, in general, signals the appearance of or change in a symmetry in the wave function, can also correspond to disordered points. In this case, however, the entropy curve does not show anomalous behavior because this is not a phase transition in the conventional sense. When the decaying correlation function has an incommensurate oscillation, a new peak appears close to $q = 0$ in the Fourier spectrum and moves towards a commensurate wave vector as the control parameter is adjusted. In the entropy of the triplet excited states, in addition to a peak at the same position as in the ground-state entropy, another peak appears at the wave vector of the peak in the static structure factor. Our method is ideal for use in conjunction with the density-matrix renormalization-group algorithm because the block entropy profile is generated as a by-product of the DMRG procedure. This allows the more difficult and sensitive calculation of correlation functions to be avoided.

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**Fig. 7:** Block entropy profile of a finite chain with $N = 64$ sites for the $t - t' - U$ Hubbard model for $U = 3$ at $t' = 0.6, 0.625, 0.65, 0.675$ (from top to bottom).

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