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 and also provide significant information about certain relevant features of the excitation spectrum; in particular, they can identify the wave vector of soft modes in critical models.

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Recently, the use of concepts of quantum information theory, such as the von Neumann entropy and other measures of entanglement between parts of a quantum system, has gained popularity in statistical physics and solid state physics. In particular, it has been shown that because these quantities exhibit discontinuities or extrema at transition points [1], they can be used to detect and locate quantum phase transitions (QPTs) that occur as the coupling constants are varied. This method has been used to study QPTs in low-dimensonal spin [2–7] and fermionic [8–12] problems.

In this Letter, we propose a new procedure which can be used to obtain additional information from the von Neumann entropy. We will show how to determine the wave vector characterizing the new phase when the system goes from a uniform to a spatially inhomogeneous phase. Similarly, if the system has soft modes, the method can extract their wave vector. Moreover, this method is well-suited for studying cases when no true phase transition takes place, but the decay of the correlation function changes character. Thus, this method provides a powerful new tool to determine the ground-state phase diagram of interacting quantum systems.

The method is based on the study of the length dependence of the von Neumann entropy of a finite segment of a one-dimensional quantum system. It is known that this quantity behaves fundamentally differently for critical and noncritical systems [13,14]. The entropy of a subsystem of length l (in units of the lattice constant a) in a finite system of length N 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 [15,16] for models that map to a conformal field theory [17]:

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

and this form has been shown to be satisfied by critical spin models. Here, c is the central charge, and g is a constant shift due to the open boundary which depends on the ground-state degeneracy. An additional alternating term, which decays as a power law, appears near the boundary [18].

The aim of this Letter 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. Oscillations may appear; if so, they can be conveniently analyzed through the Fourier spectrum of $s(l)$. The method is especially appropriate when the density-matrix renormalization-group (DMRG) algorithm [19] is used because 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.

We will first consider QPTs of the spin-one bilinear-biquadratic model [20],

$$\mathcal{H} = \sum_i [\cos\theta(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \sin\theta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \qquad (2)$$

that occur at the exactly solvable Takhtajan-Babujian (TB) [21] and Uimin-Lai-Sutherland (ULS) [22] points, corresponding to $\theta = -\pi/4$ and $\pi/4$, respectively. As usual in the DMRG approach, we consider open chains. The numerical calculations were performed using the dynamic block-state selection (DBSS) approach [23]. The threshold value of the quantum information loss χ 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 states was set to $M_{\max} = 1500$.

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.

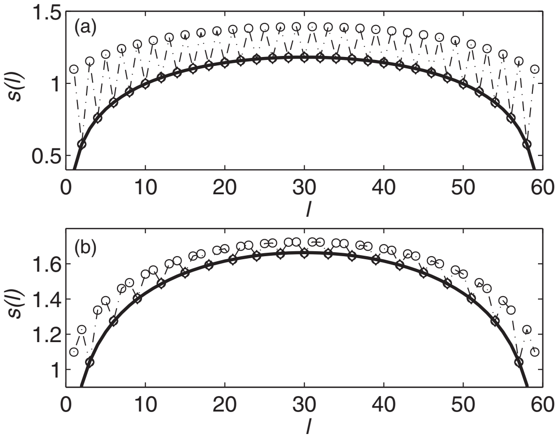

FIG. 1. Length dependence of the von Neumann entropy of segments of length l of a finite chain with $N = 60$ sites for (a) the Takhtajan-Babujian and (b) the Uimin-Lai-Sutherland models. The solid lines are our fit using Eq. (1), taking every second and third data point in (a) and (b), respectively.

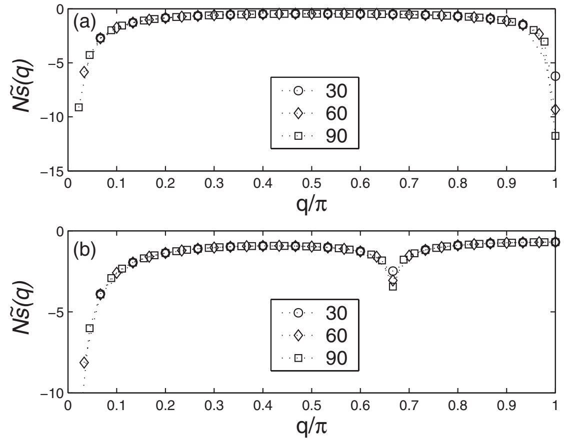

FIG. 2. Fourier spectrum $\tilde{s}(q)$ (scaled by the system size N) of the length-dependent von Neumann entropy of finite chains of length $N = 30$, 60, and 90 for (a) the Takhtajan-Babujian and (b) the Uimin-Lai-Sutherland models.

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, $c = 3/2$ [24] and $c = 2$ [25], 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 transform

$$\tilde{s}(q) = \frac{1}{N}\sum_{l=0}^{N} e^{-iql}s(l), \quad (3)$$

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 $0 \le q \le \pi$ 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 π, 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 $N \to \infty$ 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 θ in the range $-3\pi/4 < \theta < -\pi/4$, where the system is gapped and dimerized, the peak at $q = \pi$ remains finite as $N \to \infty$. On the other hand, in the whole interval $\pi/4 \le \theta < \pi/2$, where the system is gapless and the excitation spectrum is similar to that at the ULS point, the entropies for block sizes that are multiples of three can be well-fitted with the form given in Eq. (1) with $c = 2$, and for finite chains, a peak appears in $\tilde{s}(q)$ at $q = 2\pi/3$, in agreement with Refs. [20,25]. Thus, peaks in the Fourier spectrum of the length-dependent block entropy can provide useful information about the excitation spectrum and the wave vector of soft modes, even when they scale to zero in the thermodynamic limit.

We can also demonstrate this procedure near the AKLT point [26], corresponding to $\theta_{\mathrm{AKLT}} = \arctan 1/3 \simeq 0.1024\pi$. It is known [27] 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 $\theta_L = 0.138\pi$, the so-called Lifshitz point. In an earlier work [11], some of us showed that $s(N/2)$ has an extremum as a function of θ at θ_{AKLT}. Here, we show that this extremum is the indication that, in fact, θ_{AKLT} is a dividing point which separates regions with a different behavior of $s(l)$ and $\tilde{s}(q)$.

At and below the AKLT point, i.e., for $-\pi/4 < \theta \le \theta_{\mathrm{AKLT}}$, $s(l)$ increases with l for small l, saturates due to the Haldane gap [28], 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 AKLT point, depicted in Fig. 3, illustrates this behavior. For θ slightly larger than θ_{AKLT}, however, we find that $s(l)$ does not increase to the saturation value purely monotonically. Instead, an incommensurate oscillation is superimposed. For somewhat larger θ 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 θ value is slightly smaller than, but close to, the Lifshitz point.

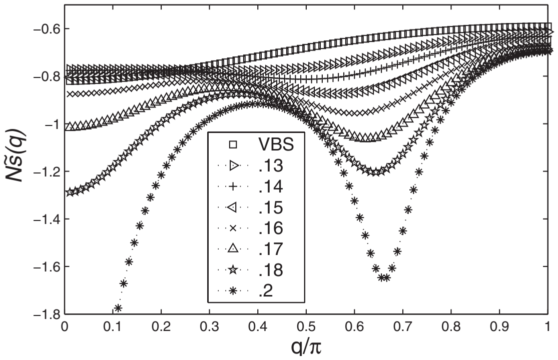

FIG. 3. Fourier-transformed entropy $\tilde{s}(q)$ for various θ, obtained for a finite chain with $N = 180$ lattice sites. The lines are guides to the eyes. The $q = 0$ point, which has a large positive value, is not shown.

It is also interesting to examine the behavior of the block entropy in the lowest-lying excited state. This is shown in Fourier-transformed representation, $\tilde{s}(q)$, in Fig. 4, for several θ values.

The appearance of the new peaks are even more pronounced, and data for $\theta < \theta_L$ confirm that this approach can probe the incommensurate phase much closer to the transition point than is possible using only the static structure factor $S(q)$. Although the new peak(s) in $\tilde{s}(q)$ in the incommensurate phase move in an opposite sense to those in $S(q)$, i.e., the peak approaches $2\pi/3$ from zero and not from π, they can be easily related to each other. By also calculating $S(q)$, we found within the error of our calculation that the location, q^*, of the peak in $\tilde{s}(q)$ is related to the wave vector q at which $S(q)$ has its maximum by $q = \pi - q^*/2$.

The spin-1/2 frustrated Heisenberg chain is also known to develop incommensurate correlations when $J'/J > 0.5$, where J is the nearest- and J' the next-nearest-neighbor coupling. We have found that 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

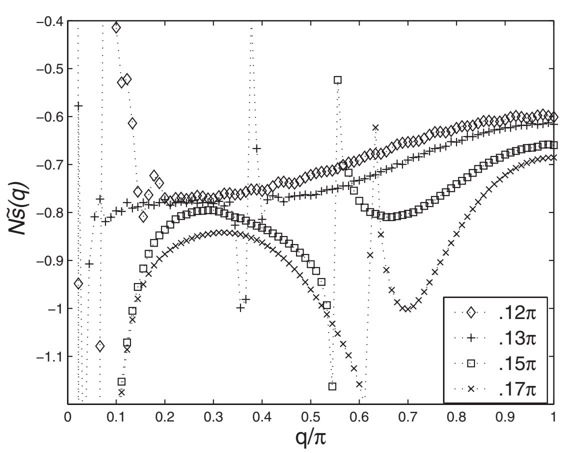

FIG. 4. Same as Fig. 3 but for the $S^z_{\mathrm{Tot}} = 2$ quintet excited state.

the Majumdar-Ghosh point [29]. Thus, the transition from commensurate (dimerized) to incommensurate correlations is marked again by an extremum of the block entropy. In the incommensurate phase, a new peak that moves from $q = 0$ towards $q = \pi/2$ appears in the Fourier spectrum. When the behavior of the block entropy in the lowest-lying triplet excited state is examined, we find two oppositely moving peaks in $\tilde{s}(q)$. One appears exactly where the peak was found for the ground state, q^*, while the other occurs at $\pi - q^*$. By also calculating $S(q)$ we have found again that, to within the error of our calculation, this second peak is located at the same (J'/J-dependent) wave vector at which $S(q)$ has its maximum [30].

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

$$\mathcal{H} = t\sum_{i\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + c^\dagger_{i+1\sigma}c_{i\sigma}) + t'\sum_{i\sigma}(c^\dagger_{i\sigma}c_{i+2\sigma} + c^\dagger_{i+2\sigma}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \quad (4)$$

which has been investigated recently [31]. 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, this transition is preceded by the opening of a spin gap at $t'_s < t'_c$. Between t'_s and t'_c, the wave vector becomes incommensurate for $t' > t'_{\mathrm{IC}}$. Thus, the commensurate-incommensurate transition is independent of the metal-insulator transition [31].

As expected for a commensurate-incommensurate transition, we find that the entropy of blocks of length $N/2$ 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 $t'_{\mathrm{IC}} \simeq 1/\sqrt{2}$, which maps to the Majumdar-Ghosh point. The block entropy is shown in Fig. 5(a) for $U = 3$, a value chosen so that our results can be directly compared to those of Ref. [31]. This shows that the transition point can accurately be detected and located on system sizes, that are typically a factor of 2 to four smaller than those needed with the standard methods used in Ref. [31]. For $t' > 0.6$, an incommensurate oscillation in $s(l)$ becomes apparent, as well as in its Fourier-transformed representation, $\tilde{s}(q)$.

When $\tilde{s}(q)$ 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 $\tilde{s}(\pi)$ 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. This phase boundary is depicted in Fig. 5(b).

In conclusion, we have shown that the length dependence of the block entropy and its Fourier spectrum, de-

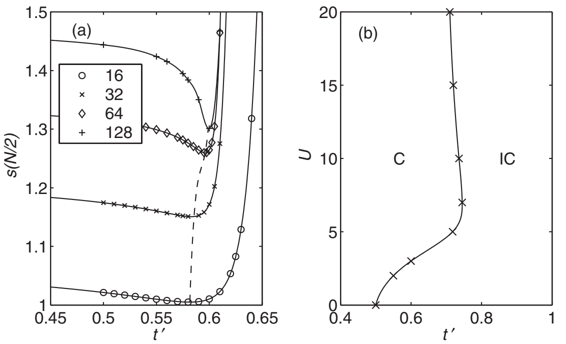

FIG. 5. (a) Entropy of blocks of length $N/2$ as a function of t' for the 1D $t - t' - U$ Hubbard model for $U = 3$ and various chain lengths. The dashed line is a spline through the minima. (b) Phase boundary of commensurate-incommensurate transition in the t'-U plane obtained from a finite-size extrapolation of the minima in (a). The line is a spline through the indicated points.

termined for finite systems, can be used to characterize phases in which the correlation function has an oscillatory character. This method also provides significant information about some features of the excitation spectrum and allows one to identify soft modes in critical models. 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 disorder 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 spin excited states, another peak can appear at the wave vector of the peak in the static structure factor, in addition to a peak at the same position as in the ground-state entropy. A simple relationship has been shown to exist between the wave vectors of the peaks of $\tilde{s}(q)$ and $S(q)$. 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 leads, on the one hand, to substantially improved sensitivity compared to the calculation of correlation functions, which depend on the accuracy of the variational wave function, or of gaps, which require the calculation of energy differences as well as a careful finite-size scaling, and, on the other hand, to qualitatively new, physically intuitive, and useful information. As this Letter was being revised, an application of this method to the SU(n) Hubbard model has appeared [32].

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