Entanglement used to identify critical systems

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(Dated: 10 March 2005)

We promote use of the geometric entropy formula derived by Holzhey et. al. from conformal field theory, \( S_\ell \sim (c/3) \log \left( \sin \frac{\pi \ell}{N} \right) \), to identify critical regions in zero temperature 1D quantum systems. The method is demonstrated on a class of one-dimensional \( XY \) and \( XYZ \) spin-\( \frac{1}{2} \) chains, where the critical regions and their corresponding central charges can be reproduced with quite modest computational efforts.

PACS numbers: 03.67.Mn, 75.10.Pq, 11.25.Hf

I. INTRODUCTION

Continuous phase transitions [1] are characterized by a diverging correlation length and the emergence of scale invariance. If the system is governed by local interactions (so that a conserved, symmetric and traceless energy-momentum tensor can be defined at the critical points) the scale symmetry is automatically enlarged to the full conformal group [2]. In two dimensions this group is infinite dimensional; this provides a lot of information about the behaviour of critical systems in two dimensions [3, 4]. One quantity which can be computed exactly by use of conformal symmetry is the entanglement entropy, i.e. the von Neuman entropy

\[
S_A = -\text{Tr} \rho_A \log \rho_A
\]

of the reduced density matrix \( \rho_A = \text{Tr}_B |\Omega\rangle \langle \Omega| \) for a subsystem \( A \) of a system \( A + B \) in the ground state \( |\Omega\rangle \).

This entanglement entropy is, in the case of pure states, a measure of the entanglement between subsystems \( A \) and \( B \) [5]. In the case where \( A \) is a segment of length \( \ell \) of a circle \( A + B \) of circumference \( N \) the result is

\[
s_\ell \equiv S_\ell - S_{N/2} = \frac{c + \bar{c}}{6} \log \left( \sin \frac{\pi \ell}{N} \right),
\]

where \( c (\bar{c}) \) is the holomorphic (antiholomorphic) central charge. This result was first derived by Holzhey et. al. [6] (denoted geometric entropy), and has recently been extended in several directions by Calabrese and Cardy [7]. The explicitly known dependence of \( s_\ell \) on the scaling variable \( \ell/N \) is a distinguishing feature of Eq. (2).

The main purpose of this note is to point out how well Eq. (2) is reproduced at critical parameters [8] , even for very small systems. The comparison of a numerical calculated \( \ell \)-dependence with this formula is in our experience a very efficient method to identify critical points. This is illustrated in Fig. 1. As can be seen the entanglement of noncritical systems saturates at finite \( \ell \) (determined by the correlation length), in contrast to critical ones which follow Eq. (2) closely. The system considered in Fig. 1 is defined by the Hamiltonian

\[
H_{\text{Ising}} = \sum_{n=0}^{N-1} \left( \sigma_n^x \sigma_{n+1}^x + \lambda \sigma_n^z \right),
\]

where periodic boundary conditions are applied, i.e., \( \sigma_N \equiv \sigma_0 \). We shall refer to it as the 1D quantum Ising model [9]. Throughout this paper logarithms are calculated base two. As can be seen the critical point can be quite accurately determined from surprisingly small systems. An additional advantage is that the analysis can be performed without varying the total system size \( N \). To further illustrate this point we have calculated the mean square deviation

\[
\varepsilon \equiv \frac{1}{M} \sum_{\ell} (\hat{s}_\ell - s_\ell)^2,
\]

where \( \ell \) runs over integers satisfying \( 0.2 N < \ell < 0.8 N \), \( M \) is the number of such integers, and \( \hat{s}_\ell \) is the quantity corresponding to Eq. (2) calculated from the ground state of a finite system with \( c = \bar{c} \) chosen to minimize \( \varepsilon \).

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Results for the quantum Ising model is shown in Fig. 2, where the critical Ising point $\lambda = 1$ is readily identified even for a system as small as $N = 10$. Using the minimal error as an estimate of the critical point we have plotted out this estimate and the corresponding error in Fig. 3, which illustrates how the identification improves with system size. In Fig. 4 we see the central charge estimates for the quantum Ising model and the correct central charge $c = \frac{1}{2}$ is readily identified for $N = 10$ system. From these results we conjecture that one may apply the formula (2) to identify critical points and the corresponding central charges by investigating systems of sizes as low as $N \simeq 10$. The main advantage of this is that we can use an exact numerical diagonalization of the Hamiltonian (possibly utilizing known information about conservation laws) to obtain critical information about a larger class of models than what is obtainable from ordinary means such as fermionizing the XY model reviewed in the next section.

It is of course well known that global system entanglement increases logarithmically at critical points [10, 11], and that this scaling can be utilized [12]. But the $\ell$-dependence reveals much more of the vast information carried by the wave function for a single system. This seems much more efficient than identifying a slow logarithmic divergence with system size.

II. THE XY AND XYZ QUANTUM SPIN CHAINS

To assure that the results shown in Figs. 1-4 are more than coincidences, we have studied a larger class of models. The general translational invariant, Hermitian spin-$\frac{1}{2}$ chain, with only local and nearest-neighbor interactions, can (with suitable coordinates) be described by the Hamiltonian

$$H = - \sum_{n=0}^{N-1} \left[ \sum_{\alpha} f_{\alpha} \sigma_n^\alpha \sigma_{n+1}^\alpha + g \cdot (\sigma_n \times \sigma_{n+1}) + h \cdot \sigma_n \right],$$

where $f$, $g$ and $h$ are real three-vectors, and $\sigma$ the Pauli spin matrices. We impose periodic boundary conditions, $\sigma_N \equiv \sigma_0$. The previously studied quantum Ising model

![FIG. 3: The estimated critical point $\lambda_c$ (+) and the corresponding deviation $\varepsilon$ (×) as function of system size $N$. The fulldrawn line is the fit $\lambda_c = 1 + 5.3715 N^{-3}$.](image3.png)

![FIG. 4: The estimated central charge $c$ for the 1D Ising model (cf. Fig. 2) obtained by fitting $c = \bar{c}$ so that $\varepsilon$ of Eq. (4) is minimized. The dashed line is for $N = 10$, the fulldrawn line for $N = 50$. The inset shows details close to the critical point in the 1 percent region. As can be seen the correct central charge is well reproduced.](image4.png)
corresponds to the case \( f_x = 1 \), \( h_z = \lambda \), with all other parameters zero. This is a special case of the two-parameter \( XY \) quantum spin chain, defined by \( f_x = (1 + \gamma)/2 \), \( f_y = (1 - \gamma)/2 \), \( h_z = \lambda \), i.e.,

\[
H_{XY} = - \sum_{n=0}^{N-1} \left( \frac{1 + \gamma}{2} \sigma_n^x \sigma_{n+1}^x + \frac{1 - \gamma}{2} \sigma_n^y \sigma_{n+1}^y + \lambda \sigma_n^z \right),
\]

(6)

which can be expressed as a quadratic form in fermion variables through a Jordan-Wigner transformation [13].

Therefore, many aspects of the \( XY \) model are exactly calculable, making it a good benchmarking tool for our method. Symmetry of the space spanned by the anisotropy parameter \( \gamma \) and magnetic field \( \lambda \) makes it sufficient to consider only the first quadrant, \( \gamma \geq 0 \), \( \lambda \geq 0 \), where the model has two critical lines (see Fig. 5). We have investigated how well the critical line of the \( XY \) model is identified for larger values of \( \lambda \) and \( \gamma \). Our findings are that the behavior at the Ising critical point is not untypical of the cases considered, but exceptions can be found. One general feature is that a minimum in \( \varepsilon \) is correlated with a maximum in the estimated central charge \( \hat{c} \), but that these two points do not coincide exactly; their difference is a possible measure of how accurate the critical point has been found. In most cases we have found the maximum in \( \hat{c} \) to lie closest to the critical point, but again there are exceptions. There is also a tendency that the maximum estimated \( \hat{c} \) slightly overshoots its exact value, but since by the Kac formula \( c \) is quantized to \( 1 - 6/m(m + 1) \) \( (m = 3, 4, \ldots) \) in unitary models with \( c < 1 \) this may be possible to correct. Due to symmetry the method identifies the \( c = 1 \) critical line \( \gamma = 0 \) exactly; however with more shallow minima in \( \varepsilon \) and a somewhat larger overshoot of \( \hat{c} \).

In Fig. 6 we show a contour plot of \( \hat{c} \) and \( \varepsilon \) over a whole region of the parameter space in the \( XY \) model, scanned for system size \( N = 12 \), as would have been realistic in a case where we had no \( a \ priori \) knowledge about the positions of the critical lines (or even their existence). Our conclusion is that such a scan locates the critical lines quite reliably; the identified regions could next be analyzed more carefully for larger system sizes. Since there is a crossover between \( c = \frac{1}{2} \) and \( c = 1 \) at \( (\gamma, \lambda) = (0, 1) \), an interesting question is how well the method works near this point. We find that the minima in \( \varepsilon \) generally split as we approach this point, probably due to competition between the two critical lines, thus creating some ambiguity. The region of ambiguity shrinks with increasing \( N \).

By adding another term to (6) we obtain the \( XYZ \) model,

\[
H_{XYZ} = H_{XY} - \sum_n \Delta \sigma_n^x \sigma_{n+1}^x.
\]

(7)

With \( \lambda = 0 \) the thermodynamics of this model has been found exactly [15], Eq. (7) then being the Hamiltonian limit of the transfer matrix of the eight-vertex model. It has a critical line given by \( \gamma = 0 \), \( |\Delta| \leq \frac{1}{2} \), and a central charge \( c = 1 \). Also in the isotropic case, \( \gamma = 0 \), the thermodynamics has been solved exactly. There is a critical surface given by \( |\lambda| \leq 1 - 2|\Delta| \) [16].

With \( \Delta \neq 0 \) the Hamiltonian (7) can no longer be transformed to a quadratic fermionic form. Thus our entanglement calculations require a more brute force numerical calculation, starting from a \( 2^N \times 2^N \) Hamiltonian matrix (which can be somewhat reduced in size by utilizing all possible symmetries) [17]. Thus the required computational resources grow exponentially with \( N \), limiting the current feasible system size to \( N = 20 \) at best.

We have analyzed various regions of the three-dimensional parameter space for \( N = 14 \) or less, and ver-
of a whole region, scanned for system size \( N = 12 \) and \( \Delta = \frac{1}{4} \). Here the most interesting feature is the identification of the \( c = \frac{1}{2} \) critical line, marked with thick lines in Fig. 7. This is a continuation of the \( \lambda = 1 \) critical line of the XY model to non-zero values of \( \Delta \), and has to our knowledge not been calculated before. In the figure we have not drawn it all the way to the point \( (\gamma, \lambda) = (0, \frac{1}{2}) \). This is to indicate the computational uncertainty which arises near this point, not to indicate that the critical line ends.

In conclusion, we have found an efficient technique to identify quantum critical regions of Hamiltonians such as (5), and others that show conformal invariance at the critical points. The method compares the entanglement entropy with the conformal scaling formula provided by Eq. (2) of Holzhey et al., and work sufficiently well for small systems to enable us to employ brute force numerical diagonalization of the Hamiltonian to identify criticality and central charges in models that are insoluble through other means such as fermionizing. The method is not limited to spin-\( \frac{1}{2} \) systems or nearest-neighbor interactions, though it may work better with shorter range of interactions (since the emergence of conformal symmetry relies on the existence of an energy-momentum tensor, i.e., on local interactions).

Acknowledgment

We thank the Department of Physics, University of Tromsø, where this work was finalized, for its generous hospitality.

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