Entanglement Entropy in Condensed-Matter Systems

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We review the application of entanglement entropy in condensed-matter systems, with focus on triangular spin lattice system of spin-1/2 and spin-1. This article is based on a series of presentations in "Student Seminar Theoretical Physics, 2016 Fall" at Utrecht University.

I. REVIEW OF ENTANGLEMENT ENTROPY

In trying to devise a measure M of entanglement in a system, it is mandatory that it obey two conditions. First, M should vanish for separable states $\rho = \rho_A \otimes \rho_B$. Second, M should be invariant under local unitary transformations, since entanglement is precisely a global feature of the system which cannot be created or altered by local transformations. The simplest measure that respects these restrictions is Entanglement Entropy (EE) of which there are two sorts: the von Neumann EE (1) , and the Rényi EE (2).

$$S_{VN}(\rho) = Tr[\rho\, log_2(\rho)] \tag{1}$$

$$S_{R,\alpha}(\rho) = \frac{1}{1-\alpha} Tr[\rho^\alpha] \tag{2}$$

It is important to note that EE measures the entanglement of the system with its exterior and not the entanglement within the system. As such if we want to quantify entanglement within a system first we need to divide it into two subsystems and subsequently compute the EE of one of the systems such that

$$E(\rho) = S(\rho_A) = S(\rho_B) \tag{3}$$

It is easily shown that EE vanishes for pure states $\rho = |\Psi\rangle\langle\Psi|$. Since a pure state cannot be entangled to any other, this is in accordance with the interpretation that EE measures the entanglement of the system with the exterior. It can also be shown that EE reaches its maximum for completely mixed states of the subsystems, i.e. the global state is maximally entangled. This is sufficient to persuade us that EE is a competent measure of entanglement.

Another very important result in the study of EE is the so called *Area Law*, which consists in the following. If we divide a system in a subsystem A and its complement then the EE of A scales with the boundary of A (4).

$$S(\rho_A) \propto \partial A \tag{4}$$

Area law is valid for ground states of local Hamiltonians, which are non generic states that occupy a small region of the whole Hilbert space.

II. EE IN 1D SYSTEMS

In order to explore applicability of the area law, we start by looking at one dimensional systems. For this, we expect that the entropy be constant (Eisert *et al.*, 2010). What we in fact observe is that it will be so for a ground state with finite correlation length, and will increase logarithmically for an infinite correlation length, or a much bigger one than the system.

For the Heisenberg and Ising models we do not observe a phase transition with a temperature-related order parameter, but we know that one of the defining features of these phase transitions, in higher dimensions, is that the correlation length becomes infinite at the phase transition point. Measuring the entanglement entropy at zero temperature in one dimension in these systems shows that we can have two regimes depending in the parameters of the model: a constant entropy or a logarithmically increasing entropy (Vidal *et al.*, 2003). Hence we conclude that we have observed a quantum (no order parameter) phase transition (we go from a finite to infinite correlation length) (Amico *et al.*, 2008). This can be related with the system being gapped (non-critical) in the constant entropy phase, with means that there is an energy cost to go from the ground state to the first excited state, or the system being gapless (or critical), where there is not such cost and can be mapped to conformal field theories, which predict the behaviors that are found (Eisert *et al.*, 2010) (Amico *et al.*, 2008) (De Chiara *et al.*, 2006). The previous description is expected to be general to all one dimensional systems, and it is conjectured that we can find a direct correspondence between gapped systems and quantum criticality (Eisert *et al.*, 2010). In higher dimensions, however, we can find several deviations, for instance that the area law depends on the fermi surface if we are dealing with a fermionic system, or that the area law holds for some bosonic systems, even after criticality (Amico *et al.*, 2008).

Experimental evidence that entanglement entropy relates with quantum phase transitions has been found by (Islam *et al.*, 2015), where they use a 4×2 lattice of ^{87}Rb atoms, and use the parity to calculate the second order Renyi entropy, which relates directly with quantum entanglement. They show that the phase transition be-

tween a Mott insulator and a superfluid is predicted by the entropy, which is bigger when we consider only part of the system than the system as a whole when we are at a strongly correlated state, the superfluid state. This experiment shows that there is a solid relation between entanglement entropy, phase transitions, and the entangled nature of the ground state for critical systems, as well as how this changes across a quantum phase transition, at least in a 1D system.

III. 2D TRIANGULAR SPIN LATTICE SYSTEMS

In many-body systems, at zero temperature, although there is no thermal fluctuation, there are still quantum fluctuations which drive the system into different phases based on other external physical parameters such as magnetic field, pressure, chemical composition, etc. These phases of matter are called quantum phases (e.g. Superconductor Insulator Transition, non-Fermi liquid (or "strange metal"), Quantum magnets, Quantum Hall system, etc. (Amico *et al.*, 2008)). Motivated by methods developed in quantum information theories (Preskill, 2016), we are going to look at the entanglement properties in the ground state of our system. From there, we can detect different quantum phases and also quantum phase transitions based on the variation of these entanglement properties. In contrast with the well-studied 1-dimensional (1D) system (Vidal *et al.*, 2003), there are much less known about higher dimensional system due to the difficulties in solving non-integrable large systems using calculation techniques such as Exact Diagonalization (ED), Quantum Monte Carlo (QMC) or Tensor Networks. Thanks to interesting features of geometric frustration system (Diep, 2013), we will focus specifically on the 2D triangular spin lattice systems in two cases of spin-1/2 and spin-1 particles.

The spin-1/2 case will be theoretically described by spin-1/2 XXZ Hamiltonian model:

$$H_{XXZ} = \sum_{\langle i,j \rangle} \left[J_\perp \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \right) + J_z \sigma_i^z \sigma_j^z \right] \qquad (5)$$

where σ^α ($\alpha = x, y, z$) are the spin-1/2 Pauli matrices and $\langle i, j \rangle$ refers to all possible pairs of first neighbors. For convenience of comparison with the spin-1 model, the parameters in the Hamiltonian are chosen without loss of generality as $J_\perp = (2\cos\theta - \sin\theta)/2$ and $J_z = \sin\theta/2$.

For the spin-1 case, we have the following Heisenberg Bilinear-Biquadratic (BB) Hamiltonian:

$$H_{BB}(\theta) = \cos\theta \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \sin\theta \sum_{\langle i,j \rangle} \left(\vec{S}_i \cdot \vec{S}_j \right)^2 \qquad (6)$$

where now $\vec{S} = (S_x, S_y, S_z)$ are the spin $S = 1$ operators.

Based on parameter θ described in the Hamiltonian models, there will be 5 different phases for spin-1/2 case, as shown in Figure 1: *FerroMagnetic* along $\hat{z}$-axis (FMz) for $\theta \in (\pi/2, 5\pi/4)$, *FerroMagnetic* in $\hat{x}\hat{y}$-plane (FMxy) for $\theta \in (5\pi/4, \Theta_{XXZ})$, *Supersolid* (SS1) for $\theta \in (\Theta_{XXZ}, 0)$, *Supersolid* (SS2) for $\theta \in (0, \pi/4)$, and *AntiferroMagnetic* (120°-Néel in the $\hat{x}\hat{y}$-plane) (AFM) for $\theta \in (\pi/4, \pi/2)$

Meanwhile, there are four locally ordered phases for spin-1 case as seen in Figure 1: *FerroMagnetic* (FM) for $\theta \in (\pi/2, 5\pi/4)$, *FerroQuadrupolar* (FQ) for $\theta \in (5\pi/4, \Theta_{BB})$, *AntiferroMagnetic* (AFM) for $\theta \in (\Theta_{BB}, \pi/4)$, and *AntiferroQuadrupolar* (AFQ) for $\theta \in (\pi/4, \pi/2)$.

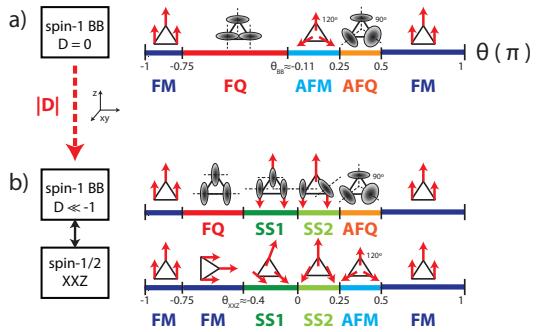

FIG. 1 Sketch of the phase diagram for the analyzed spin models: a) Spin-1 Bilinear-Biquadratic (BB) model at $D = 0$, and b) Spin-1/2 XXZ model. The spin-1 BB model in the very large easy-axis anisotropy limit ($D \ll -1$) exactly maps onto the spin-1/2 XXZ model (Moreno-Cardoner *et al.*, 2014a).

In next section, we will introduce, apply and compare 2 different computational techniques: Exact Diagonalization (ED) and a rather recently introduced technique called Cluster Mean Field (CMF) (Moreno-Cardoner *et al.*, 2014b; Yamamoto, 2009; Yamamoto *et al.*, 2012) to detect different quantum phase transitions manifested in our small (up to 12 sites) systems. There is an important

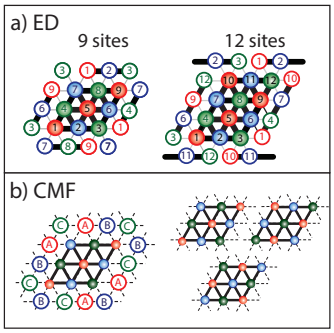

FIG. 2 Cluster sizes and geometries used in: (a) Exact diagonalization with boundary conditions as depicted, (b) Cluster Mean Field approach. Different colors indicate the three-sublattice structure. Solid lines represent quantum mechanical bonds and dashed lines the mean-field interaction between clusters.Right-bottom: non-equivalent cluster configurations for 9 sites (Moreno-Cardoner *et al.*, 2014a).

relationship between degeneracies of entanglement spec-

trum to the underlying symmetries of the system. However, in 2D system, the emergence or vanishing of these degeneracies is strongly depends on the way the partition is made. In comparison with entanglement entropy (EE) as the usual choice of global entanglement measure in 1D system, we found that in 2D triangular spin lattice system, the geometry entanglement (GE) first introduced by (Shimony, 1995) is more suitable to detect quantum phase transitions due to its insensitivity to the chosen cuts of the system.

IV. EE IN 2D TRIANGULAR LATTICES

A. Exact Diagonalization (ED)

Exact diagonalization is the most intuitive method, as it fully computes the ground state and uses it to compute everything else(Zhang and Dong, 2010).

The next step is performing a partial trace on the density of states. This can be achieved using an *a priori* defined function that finds all the associated states from the original ρ that need to be summed for a specific ρ_A entry.

The maximum value for the EE is originated by a maximal entangled state. The usefulness of EE_{max} is that it allows one to compare EE from different partition sizes. By normalizing it, one would expect all of them to overlap, regardless of partition size. As we will see in FIG. 6 on the following page that is clearly not the case, and the motive for that has to be more closely examined (Amico *et al.*, 2008).

B. Cluster Mean Field (CMF)

This method consists in dividing the lattice in clusters of 3 sites and then operate on a mean field assumption, *i.e.* treats the interactions between neighboring clusters as external fields, computed as thermodynamical expectation values using the local cluster Hamiltonian.

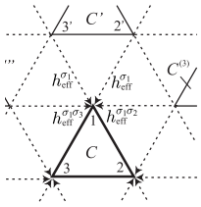

FIG. 3 CMF scheme for the triangular lattice, including how the external fields are perceived by each site in a certain cluster C (Yamamoto, 2009)

Using the layout in FIG. 3, one can establish a set of self-consistent equations (Equation (7)).

$$H_C = -J \sum_{<i,j>\in C} \sigma_i\sigma_j - J \sum_{i,i'\in C} \left(h_{eff}^{\sigma_i} + h_{eff}^{\sigma_i\sigma_{i'}}\right)\sigma_i \quad (7)$$

This generates a set of 6 non-linear equations with 6 unknowns $(h^+, h^-, h^{++}, h^{+-}, h^{-+}, h^{--})$ which can be solved numerically.

Although this method uses a mean field approximation, it can achieve a high accuracy and qualitative resemblance to ED. One of the most relevant advantages of the CMF approach is that contrary to ED, the problem size doesn't scale as 4^N. The trade-off is that numerically stable solutions can be be hard to achieve in some systems.

C. EE results for the triangular lattice

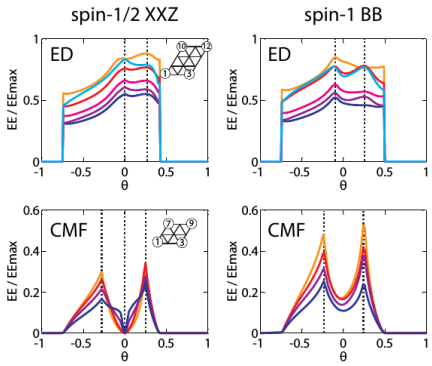

FIG. 4 Normalized EE for different partitions, using both outlined methods by (Moreno-Cardoner *et al.*, 2014a)

There are local maxima at points corresponding to second order phase transitions and discontinuities at first order phase transition points. The CMF computation signals the 2 super solid states, performing better than its ED counterpart.

D. ED calculation for the Triangular Chain

When attempting to employ our own version of the ED method, we struggled with the computation time required for a $N = 9$ simulation. Hence, we decided to make it more practical and explore the entanglement in a $N = 6$ lattice with limited periodic boundaries (FIG. 5).

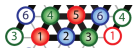

FIG. 5 Periodic boundary conditions for the triangular chain lattice

This number of interactions of each site makes this system analogous to a periodic 1D chain with interactions

between nearest and second nearest neighbors. But the arrangement of those interactions is not the same. Studying EE in this system allows one to check whether or not geometry, coordination number are relevant to the actual entanglement and to find the actual dimensionality of the system, assuming the area law holds.

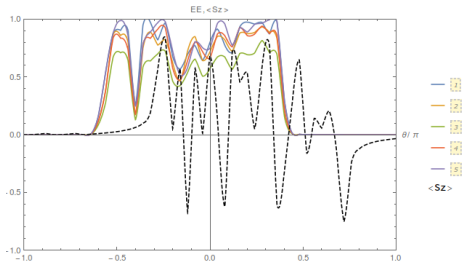

FIG. 6 ED calculation with different partition sizes for the triangular chain plotted along the magnetization

The results shown on FIG. 6 are qualitatively similar to those in FIG. 4 on the previous page. The most interesting point is that our simulation clearly points to a phase transition at θ_{XXZ} which were only present in CMF's calculations and in ED were non-existent. Unfortunately, we could not reach any reasonable explanation for this.

V. OUTLOOK

The boundary law is violated for conformal theories in one spatial dimension and is replaced by a logarithmic dependence $S \sim L^{d-1} \log L$. However, conformal theories in higher dimensions so far do satisfy the linear area law. It has been discovered that free fermions with a well defined Fermi surface violate the area law in more than one dimension (Marcos Rigol, 2006). A $d-1$ dimensional Fermi surface has an extra logarithmic scaling of the EE. Gapped fermionic systems and gapless fermionic systems with higher dimensional Fermi surfaces do obey the area law. It is now an interesting question which other systems might violate the boundary law and what this system property can be used for. Other predictions of systems violating the area law are Fermi liquids and d-wave Bose liquid phases. Frustrated quantum magnets where the low energy description is in terms of deconfined spinons with a Fermi surface should also violate the boundary law.

Another promising application is the area law violating term appearing across quantum phase transitions(A. Osterloh, 2002) (Shi-Jian Gu and Lin, 2004). More generally, EE may be used as a probe to detect topological properties of quantum many-body systems. A current field of research is the classifying of topological phase transitions. Once the universality class of the transition is characterized by determining the relevant critical exponents, the universal behavior of the entanglement entropy after the phase transition may be predicted.

Entanglement Entropy also has shown promise in the field of non-equilibrium quantum dynamics. For closed non-equilibrium systems, it has been shown that entanglement entropy can grow in time (indefinitely in infinite systems)(Weifei Li, 2008). This is significant because it leads to thermalization in the closed systems: local measurements in these systems will show a non-thermal entropy. Important questions for future research are how entanglement entropy plays a role in the dynamical properties of closed non-equilibrium systems.

REFERENCES

A. Osterloh, G. F. R. F., L. Amico (2002), Nature **416**, 608.
Amico, L., R. Fazio, A. Osterloh, and V. Vedral (2008), Rev. Mod. Phys. **80**, 517.
De Chiara, G., S. Montangero, P. Calabrese, and R. Fazio (2006), Journal of Statistical Mechanics: Theory and Experiment **2006** (03), P03001.
Diep, H. (2013), *Frustrated spin systems* (World Scientific).
Eisert, J., M. Cramer, and M. B. Plenio (2010), Reviews of Modern Physics **82** (1), 277.
Islam, R., R. Ma, P. M. Preiss, M. E. Tai, A. Lukin, M. Rispoli, and M. Greiner (2015), Nature **528** (7580), 77.
Marcos Rigol, M. O., Vanja Dunjko (2006), Phys Rev B **74** (073103).
Moreno-Cardoner, M., S. Paganelli, G. D. Chiara, and A. Sanpera (2014a), Journal of Statistical Mechanics: Theory and Experiment **2014** (10), P10008.
Moreno-Cardoner, M., H. Perrin, S. Paganelli, G. De Chiara, and A. Sanpera (2014b), Phys. Rev. B **90**, 144409.
Preskill, J. (2016), California Institute of Technology.
Shi-Jian Gu, Y.-Q. L., Shu-Sa Deng, and H.-Q. Lin (2004), Physical Review Letters **93** (086402).
Shimony, A. (1995), Annals of the New York Academy of Sciences **755** (1), 675.
Vidal, G., J. I. Latorre, E. Rico, and A. Kitaev (2003), Phys. Rev. Lett. **90**, 227902.
Weifei Li, R. Y. T. R. S. H., Letian Ding (2008), Nature **452**, 854.
Yamamoto, D. (2009), Phys. Rev. B **79**, 144427.
Yamamoto, D., A. Masaki, and I. Danshita (2012), Phys. Rev. B **86**, 054516.
Zhang, J., and R. Dong (2010), European Journal of Physics **31** (3), 591.