

Mean-field approximations and multipartite thermal correlations

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Abstract. The relationship between the mean-field approximations in various interacting models of statistical physics and measures of classical and quantum correlations is explored. We present a method that allows us to find an upper bound for the total amount of correlations (and hence entanglement) in a physical system in thermal equilibrium at some temperature in terms of its free energy and internal energy. This method is first illustrated by using two qubits interacting through the Heisenberg coupling, where entanglement and correlations can be computed exactly. It is then applied to the one-dimensional (1D) Ising model in a transverse magnetic field, for which entanglement and correlations cannot be obtained by exact methods. We analyse the behaviour of correlations in various regimes and identify critical regions, comparing them with already known results. Finally, we present a general discussion of the effects of entanglement on the macroscopic, thermodynamical features of solid-state systems. In particular, we exploit the fact that a d -dimensional quantum system in thermal equilibrium can be made to correspond to a $(d + 1)$ -dimensional classical system in equilibrium to substitute all entanglement for classical correlations.

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1. Introduction

Entanglement is an effect that has been studied extensively since 1935, when Einstein, Podolsky and Rosen and (independently) Schrödinger introduced it as a purely quantum phenomenon without any counterpart in classical physics. Although counterintuitive by its nature, entanglement is a real physical effect that has been experimentally demonstrated through violation of Bell's inequalities, experiments on teleportation, dense coding and entanglement swapping. Most recently, entanglement has been shown to affect macroscopic properties of solids, such as its magnetization and heat capacity [1]. This effect is observed only at low temperature; nevertheless, it is still impressive that a virtually macroscopic system can feel the effects of purely quantum correlations. The purpose of this paper is to explore a general method of quantifying and bounding total correlations in any such physical system.

Extensive effort has been made to understand theoretically and to quantify entanglement [2]. A large number of different measures have been proposed. However, we have recently argued that, based on the very natural local processes and classical communication, we should not expect to find a unique measure of entanglement even for mixed bipartite states [3]. Therefore, different measures capture different aspects of entanglement, but no measure can capture all aspects. This apparent ambiguity will not present a problem for us here as will be seen shortly.

The main purpose of this paper is to study multipartite thermal entanglement in general solid state systems. Many investigations have recently been conducted in this direction [4]–[15], and entanglement is found to be present under some circumstance and has been linked to the existence of critical phenomena. However, all of the work so far uses some form or other of bipartite measures of entanglement. This is because we have an almost complete understanding of bipartite entanglement and can even compute its amount exactly. In this paper, on the other hand, we will be addressing genuine multipartite correlations. The measure that we will use is the relative entropy of entanglement which is the only current measure that can be consistently used for any number of particles and dimensions.

The key result of this paper will be a derivation of an upper bound on the amount of total correlation in a thermal state of any macroscopic system. This will, of course, be a bound on the amount of entanglement as well, since entanglement is a special case (i.e. the quantum part) of correlations. We will apply the derived bound to two simple interacting systems of qubits and

analyse the limitations of our method. Interestingly, in spite of the bound not being exact, we are still able to see regions of criticality. At the end, we will discuss the correspondence between a d -dimensional quantum-interaction systems and $(d + 1)$ -dimensional classical systems and examine its implications on the existence of macroscopic thermal entanglement.

We introduce now the measures of information that will be used throughout. We first introduce the quantum (von Neumann) mutual information, which refers to the correlation between two quantum subsystems. The quantum mutual information between the two subsystems ρ_1 and ρ_2 of the joint state ρ_{12} is defined as

$$I(\rho_1 : \rho_2; \rho_{12}) = S(\rho_1) + S(\rho_2) - S(\rho_{12}), \quad (1)$$

where $S(\rho) = -\text{tr} \rho \ln \rho$ is the von Neumann entropy. The fact that this quantity can be interpreted as a distance between the two quantum states ρ_1 and ρ_2 will be very useful for our purpose. We define the quantum relative entropy, in direct analogy with the classical (Shannon) relative entropy [2]. The quantum relative entropy between the two states σ and ρ is defined as

$$S(\sigma || \rho) = \text{tr}\{\sigma(\ln \sigma - \ln \rho)\}. \quad (2)$$

This measure has a very important application in statistical discrimination of the two states, but this role will not be of concern to us here (see [2]). What is important is that the quantum mutual information can be understood as a distance of the state ρ_{12} to the uncorrelated state $\rho_1 \otimes \rho_2$,

$$I(\rho_1 : \rho_2; \rho_{12}) = S(\rho_{12} || \rho_1 \otimes \rho_2),$$

where $\text{tr}_1 \rho_{12} = \rho_2$ and $\text{tr}_2 \rho_{12} = \rho_1$. The larger this value, the more correlated will be the state ρ_{12} . The main advantage of looking at the mutual information as a distance measure is that it can be generalized in this way to many particles. Another advantage is that it can be applied to quantify multipartite entanglement [2] as will be seen later. This applicability to many particles is precisely what we need to be able to quantify correlations in a large (macroscopic) piece of solid (in the thermodynamical limit, when the number of constituents tends to infinity). A completely uncorrelated state of n systems would be of the form $\rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_n$, and the difference between a given state ρ and this state would represent the amount of correlation present. So, the multiparty mutual information is given by [2]

$$I(\rho_1 : \rho_2 : \cdots \rho_n; \rho) = S(\rho || \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_n) = \sum_i S(\rho_i) - S(\rho). \quad (3)$$

Note that only the individual entropies and the total entropy are involved in this calculation. There is no need to look at the two, three or more subsystems and their entropies. Note also that this presents an upper bound to total entanglement in the state ρ . Intuitively speaking, this is because entanglement is only a part of the total correlations, and so it has to be smaller than the total correlations. Mathematically, we will show this in the text below.

We would like to discuss the role that these measures of information play in various models of interacting systems in statistical physics. Before we do that, we first review how entropies can be used to generalize and formalize the notion of the mean-field approximation.

2. Mean-field approximation

The term ‘mean-field approximation’ can have various meanings in statistical mechanics and it actually refers to a whole set of different approximations all with different levels of accuracy (due

to Weiss, Bethe and others, see [16]). The main idea is to ignore the fact that the constituents of the solid under investigation are interacting and treat the interaction as an ‘average effect’. The difference between approximations lies in the way we perform the averaging. In this section we explain one method of doing so that will be used later in the paper. The aforementioned bound presented here will, however, be valid for any mean-field approximation. We will discuss the limits and failures of this method in section 6, but for a general discussion of the limits of any mean-field approximation see [16]. We would like to stress that we will not at all make any new contribution here to the mean-field approximation; our aim is to use the existing theory to quantify multipartite correlations.

The key quantity in statistical mechanics that allows us to derive thermodynamical properties of the system under study is free energy. Once this quantity is known, we can, by differentiation with respect to suitable parameters, derive all other thermodynamical variables, such as pressure, energy, magnetization and so forth. The free energy is defined as

$$F = -kT \ln Z, \quad (4)$$

where k is the Boltzmann constant, T the temperature and Z the partition function. To calculate the partition function, we need to know the energy levels of the system E_i and then perform the following sum over states:

$$Z = \sum_i e^{E_i/kT}. \quad (5)$$

If the state we are considering is a quantum mechanical density matrix in a thermal state, then the partition function is given by

$$Z = \text{tr} e^{-\beta H}, \quad (6)$$

where H is the Hamiltonian and $\beta = 1/kT$. Here we will be examining only quantum models, and hence this is the expression of the partition function used. The partition function is easy to calculate if the energy levels are known, but for most of the interesting cases this cannot be done exactly. Hence various approximations had to be used. Before going into the general theory of calculation of Z , we first present a very simple example, to illustrate the main point.

Interacting systems are frequently very difficult to treat in statistical mechanics simply because there are no known analytic methods for evaluating the partition function in general. Therefore, we most often have to resort to some kind of approximation. One of the well-known ways of doing this is to write the Hamiltonian of the interacting system as a sum of non-interacting Hamiltonians for individual spins. The effect of interaction is incorporated into the average field produced by all the other spins. The method is illustrated for a simple one-dimensional (1D) Ising model.

The Hamiltonian for this model is given by

$$H = -\frac{J}{2} \sum_{i=1}^N \sigma_i^z \otimes \sigma_{i+1}^z - B \sum_{i=1}^N \sigma_i^z. \quad (7)$$

This model has been widely used to investigate various properties of real solids [16]. It can be solved exactly, but for purposes of clarity, we will illustrate it using the mean-field approximation. The mean-field Hamiltonian is

$$H_{MF} = -\frac{J}{2} \sum_{i=1}^N s \sigma_i^z - B \sum_{i=1}^N \sigma_i^z, \quad (8)$$

where s is the mean value of the neighbouring spins and there are two of them (but we also divide by 2 to avoid double counting!). This Hamiltonian is of course much easier to treat than the original one and its eigenvalues can be also immediately found to be $\pm(sJ/2 + B)$. Therefore it is easy to obtain the mean-field partition function and hence also all the other thermodynamical properties, which is why the mean-field approximation is so extensively used.

But, how do we find the value of s which is necessary for using this approximation? The value of s is given by $s = \text{tr}(\sigma^z H)$, but we have assumed that H is difficult to handle. So, instead, we use the following formula

$$s = \text{tr}(\sigma^z H_{MF}), \quad (9)$$

since H_{MF} is very easy to handle. The dipole s for this case really points in the z direction only, because we are considering a simple system. In the subsequent sections we will have to compute averages of other Pauli operators as well. This will result in a transcendental equation and for this problem in particular we have that

$$s = \tanh \frac{(Js/2 + B)}{kT}, \quad (10)$$

which cannot be solved analytically. When the external field is absent ($B = 0$), the equality can be maintained only for some range of values of J . In fact, this range is $J/2 > kT$, which leads to a critical temperature of $T_c = J/2k$. Of course, 1D models do not have phase transitions, and so the mean field incorrectly predicts the existence of the critical temperature, but nevertheless, in general this approximation turns out to be useful (especially in higher dimensions [16]). We will use it to give us an upper bound on the amount of correlations and entanglement present in interacting systems.

For convenience we will use the following dimensionless quantities in the paper: $C = B/kT$ and $K = J/2kT$. Note that this will imply, for example, that the limit of C becoming large can be reached in two different ways: B fixed and temperature tending to zero, or, T fixed and B increasing to infinity. Although these are different physically, they will invariably lead to the same result simply because only the ratio of the field strength and temperature will appear in the formulae and the two quantities never appear independently. We first discuss an important application of relative entropy to mean-field theory.

3. Bogoliubov re-derived

We describe for the sake of completeness a general method for approximating the free energy which is due to Bogoliubov. We will be interested not so much in his method for computing the free energy but the way in which it can provide us with an upper bound on total correlations in the system and hence its entanglement. Needless to say, this was not Bogoliubov's original motivation.

We start from the fact that the relative entropy is always a positive quantity,

$$S(\rho || \rho_{MF}) \geq 0, \quad (11)$$

where (in this paper) we specialize to thermal states of the form $\rho = e^{-\beta H}/Z$ and $\rho_{MF} = e^{-\beta H_{MF}}/Z_{MF}$. The entropy of both of these matrices is easy to compute. For example,

$$S(\rho) = -\text{tr} \frac{e^{-\beta H}}{Z} \ln \frac{e^{-\beta H}}{Z} = +\ln Z - \beta \text{tr}(H\rho). \quad (12)$$

Note that the last term in the above equation is just β times the average value of energy $\langle H \rangle_H = \text{tr}(H\rho)$. The subscript H in our notation means that the average is calculated with respect to the state ρ which is a thermal state generated by the Hamiltonian H . It is now straightforward to see how to compute the relative entropy between the real and mean-field thermal states. After a short calculation we have

$$S(\rho || \rho_{MF}) = \ln Z_{MF} - \ln Z + \beta \langle H_{MF} - H \rangle_H, \quad (13)$$

where, as discussed before, $Z_{MF} = \text{tr} e^{\beta H_{MF}}$. From the positivity of the relative entropy we therefore conclude that

$$0 \leq \ln Z_{MF} - \ln Z + \beta \langle H_{MF} - H \rangle_H. \quad (14)$$

This is one of the Bogoliubov inequalities. For completeness, we also derive its ‘mirror image’. Namely, we can always use the relative entropy the other way round $S(\rho_{MF} || \rho) \geq 0$, which then implies that

$$0 \leq \ln Z - \ln Z_{MF} + \beta \langle H - H_{MF} \rangle_{H_{MF}}. \quad (15)$$

We can combine the two inequalities into a single expression to obtain

$$\beta \langle H - H_{MF} \rangle_H \leq \ln Z_{MF} - \ln Z \leq \beta \langle H - H_{MF} \rangle_{H_{MF}}. \quad (16)$$

We can also express this inequality via the free energy, $F = -\ln Z/\beta$, in which case we obtain the so-called Bogoliubov inequalities:

$$\beta \langle H_{MF} - H \rangle_{H_{MF}} \leq F - F_{MF} \leq \beta \langle H_{MF} - H \rangle_H. \quad (17)$$

The purpose of this expression is the following. Suppose that we wish to approximate the partition function (or alternatively the free energy) because the exact expression cannot be easily computed. This implies that ‘free’ parameters in the mean-field Hamiltonian should be varied so that the expression $F_{MF} + \beta \langle H_{MF} - H \rangle_H$ is minimized. Since this expression has as its lower bound the true value of the free energy (this is the statement of the Bogoliubov inequality), it means that by finding the minimum we are performing the best possible approximation (within this method, of course). We can alternatively maximize the left-hand side. This method is very general and has been used many times since exactly solvable models are very rare in statistical mechanics. We will not be directly using this bound here, but will instead show how to use it to determine the upper bound for the amount of correlations in any thermal state.

4. Multipartite relative entropy of entanglement

We will now apply the formalism presented above to put a bound on the multipartite mutual information and entanglement using the free energy and internal energy. This will allow us to establish a relationship between the observable, macroscopic thermodynamical quantities and the amount of correlations in a given solid.

As we have already stated, once we have the partition function all other thermodynamical quantities can be derived [16]. For example, the magnetic susceptibility is given by

$$\chi = \frac{\partial^2 \ln Z}{\partial B^2}. \quad (18)$$

This quantity tells us the change in magnetization of the material as the external field B is increased. Microscopically, we have that the susceptibility is, in fact, a sum over all microscopic spin correlation functions

$$\chi = \sum_{ij} \xi_{ij}, \quad (19)$$

where ξ_{ij} is the spin correlation function between the sites i and j . This is a very important relation as it connects a macroscopic quantity χ to its microscopic roots in the form of the two-site correlation functions ξ_{ij} . We will show how entanglement, which fundamentally exists at the level of the microscopic correlation function, can ‘propagate’ its effects to the macroscopic level of χ . We will not be using the quantity ξ_{ij} in any fundamental way in the paper so we will not give its precise definition. Suffice it to say that any other thermodynamical quantity can in a similar way be derived from the free energy (partition function) and the interested reader is advised to consult any textbook on statistical mechanics [16]. Here we will only be concerned with multiparty correlations whose link to thermodynamics is much clearer than that of two-site entanglement.

We now define a particular measure of entanglement that has been extensively used in the literature [2] and is also appropriate for our considerations. If \mathcal{D} is the set of all disentangled (separable) states (of the form $\sum_i p_i \rho_1^i \otimes \rho_2^i$, where p_i are some probabilities), the measure of entanglement for a state σ is then defined to be the relative entropy of entanglement

$$E(\sigma) := \min_{\rho \in \mathcal{D}} S(\sigma \parallel \rho), \quad (20)$$

where $S(\sigma \parallel \rho)$ is the quantum relative entropy defined in equation (2). This measure tells us that the amount of entanglement present in the state σ is equal to its distance from the disentangled set of states. Note that this definition is, in spirit, a direct generalization of the mutual information. Whereas mutual information measures the distance of the state to the closest uncorrelated state, the relative entropy of entanglement measures its distance to the closest classically (but not quantum-mechanically) correlated state. It is therefore immediately clear that $E(\sigma) \leq I(\sigma)$ (by definition).

We will now use the equation that we introduced in the previous section

$$S(\rho \parallel \rho_{MF}) = \ln Z_{MF} - \ln Z + \beta \langle H_{MF} - H \rangle_H \quad (21)$$

to show to what extent susceptibility is dependent on entanglement. Our consideration is completely general and can be applied in any situation in statistical mechanics. Suppose that the mean-field theory gives us the closest separable state ρ_{MF} . This is not a very good assumption in general as the state in mean-field theory will be completely uncorrelated and a separable state can still have some classical correlations. This, in fact, is the advantage of the mean-field approach: by neglecting correlations we can write a Hamiltonian whose spectrum is much easier to find (it boils down to diagonalizing a 2×2 matrix for the 1D Ising and Heisenberg models). However, for the sake of argument, if the mean field gives us the closest separable state, then from the above equality we can conclude that

$$E(\rho) = \ln Z_{MF} - \ln Z + \beta \langle H_{MF} - H \rangle_H. \quad (22)$$

This is a very convenient expression since it reduces the total amount of entanglement in the state ρ to calculations of the energy and free energy of the state and its mean-field approximation.

Moreover, by differentiating twice with respect to B we can conclude that

$$\xi_{Sep} - \xi = \frac{\partial^2 E(\rho)}{\partial B^2} + \beta \frac{\partial^2 \langle H_{MF} - H \rangle_H}{\partial B^2}. \quad (23)$$

Therefore the difference in the susceptibilities between our approximation and the true value is directly proportional to (the second derivative of) the amount of entanglement in the state ρ . It is thus clear that, in general, this entanglement will have macroscopic effect on quantities such as the susceptibility (as well as other quantities). This offers a more general and formal theoretical justification for the observations in [1].

Although this equality is very suggestive from the conceptual perspective, it is most likely useless from the practical point of view for computing the amount of entanglement. This is because it is very difficult to compute the form of the closest separable state to a given entangled state. What is possible, and also very useful, will be to calculate the mean-field approximation.

So, in general, our approximation to ρ is not likely to be the closest separable state, but some completely uncorrelated state instead. Then we have the following inequality:

$$E(\rho) \leq \ln Z_{MF} - \ln Z + \beta \langle H_{MF} - H \rangle_H. \quad (24)$$

This is an upper bound on the amount of entanglement whatever be the value of ρ_{MF} we may choose. In fact, the right-hand side will more appropriately be describing the total multipartite mutual information. We would like to illustrate the usefulness of this formalism using the 1D Ising model in a transverse field. Before that, we analyse a much simpler model of two qubits interacting through an Heisenberg coupling.

5. Simple example: two qubit antiferromagnetic Heisenberg model

Thermal entanglement properties of two qubits coupled through a Heisenberg interaction are very easily understood. The Hamiltonian for the 1D Heisenberg chain in a constant external magnetic field B is given by

$$H = \sum_{i=1}^2 \left(B \sigma_i^z + \frac{J}{2} \vec{\sigma}_i \cdot \vec{\sigma}_{i+1} \right), \quad (25)$$

where $\vec{\sigma}_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$ with $\sigma_i^{x/y/z}$ being the Pauli matrices for the i th spin. The regimes $J > 0$ and $J < 0$ correspond to the antiferromagnetic and the ferromagnetic cases respectively. The state of the above system at thermal equilibrium (temperature T) is $\rho = e^{-H/kT}/Z$ where, as before, Z is the partition function and k the Boltzmann constant. The factor half in $J/2$ is added for consistency reasons with the later notation.

We first examine the two qubit antiferromagnetic chain. Since this is only a two qubit mixed state we can compute entanglement of formation exactly. We can also compute the mutual information exactly and so, there is no need to use any approximate methods. However, we will use the bound previously derived just to illustrate the method and compare it to the exact values. Before that, we review the exact results following the work of Arnesen *et al* [7].

For $B = 0$, the singlet is the ground state and the triplet states are the degenerate excited states. In this case, the maximum entanglement is at $T = 0$ and it decreases with T due to mixing of the triplets with the singlet. For a higher value of B , however, the triplet states split, and

$|00\rangle$ becomes the ground state. In that case, there is no entanglement at $T = 0$, but increasing T increases entanglement by bringing in some singlet component into the mixture. On the other hand, as B is increased at $T = 0$, the entanglement vanishes suddenly as B crosses a critical value of $B_c = 2J$ when $|00\rangle$ becomes the ground state. This special point $T = 0$, $B = B_c$, at which entanglement undergoes a sudden change with variation of B , is the point of a *quantum phase transition* (phase transitions taking place at zero temperature due to variation of interaction terms in the Hamiltonian of a system). Note that this is, strictly speaking, not a real phase transition which can only appear in the infinite- N limit. This is because, for any finite N , entanglement functions (as well as all the other thermodynamic functions) are analytic. At any finite T , however, entanglement decays off analytically after B crosses B_c . In the ferromagnetic case, the state of the system at $B = 0$ and $T = 0$ is an equal mixture of the three triplet states. This state is disentangled. Increasing B increases the proportion of $|00\rangle$ in the state which cannot make it entangled. Increasing T increases the proportion of singlet in the state which can only decrease entanglement by mixing with the triplet. Thus we never find any entanglement in the two-qubit ferromagnet. These features of the two-qubit Heisenberg model are also present in the N -qubit model [7].

Let us now apply the bound previously derived and see how well it agrees with the exact results. This is, of course, just an exercise in computing and testing the bound rather than having any practical purpose. It is convenient to do it simply because we have all the results we need and the model is really very easy to understand. On the other hand, it captures some important features of more complicated models and, therefore, it will prepare us for the next section. It is of great importance to note that the eigenvalues of the thermal state are easily found to be $2B + J/2$, $J/2$, $-2B + J/2$, $-3J/2$, the first three corresponding to the triplet states and the last to the singlet state. The partition function is then computed to be

$$Z = 2(e^{-K} \cosh 2C + e^K \cosh 2K). \quad (26)$$

In order to compute the bound, the second step is to establish the mean-field Hamiltonian. One possibility is the Hamiltonian of the form

$$H_{MF} = \left(B + \frac{J}{2} s_z \right) \sigma_z + s_x \frac{J}{2} \sigma_x + s_y \frac{J}{2} \sigma_y \quad (27)$$

for each of the two spins. The total Hamiltonian is just the sum of the above for each of the spins, and the values $s_{x,y,z}$ are the mean-field average values of the spin in the x , y and z direction, respectively. The eigenvalues of the mean-field Hamiltonian are $\pm \sqrt{(B + s_z J)^2 + (s_x^2 + s_y^2) J^2}$. The corresponding partition function is then easily computed to be

$$Z_{MF} = \left(2 \cosh \sqrt{(C + s_z K)^2 + (s_x^2 + s_y^2) K^2} \right)^2. \quad (28)$$

The ultimate square in the expression comes from the fact that there are two spins and each has the same identical individual partition function. The final quantities we have to calculate are the averages of the two Hamiltonians. We obtain for the average of H ,

$$\beta \langle H \rangle_H = \frac{1}{Z} \{ (2C + K) e^{-(2C+K)} + K e^{-K} + (-2C + K) e^{-(-2C+K)} + (-3K) e^{3K} \}. \quad (29)$$

On the other hand, we can also calculate the average mean-field energy to be

$$\beta \langle H_{MF} \rangle_H = \frac{-1}{Z} \{2(C + K s_z) e^{-K} \sinh(2C)\}. \quad (30)$$

We now estimate the average spin values $s_{x,y,z}$. This is done by computing the averages of the corresponding Pauli operators for the mean-field state. Strictly speaking, the averages should be computed with respect to the original state ρ , but this is in practice difficult to handle and it is the reason for using the mean-field approximation in the first place. Thus we have to settle for computing the following averages $\langle \sigma_x \rangle_{MF} = \langle \sigma_y \rangle_{MF} = 0$ and

$$s_z = \langle \sigma_z \rangle_{MF} = -\frac{e^{-K} \sinh(2C)}{2(e^{-K} \cosh 2C + e^K \cosh 2K)}. \quad (31)$$

Therefore only the average in the z direction is non-zero. Here we are somewhat unusually lucky since there is no s_z variable on the right-hand side. Therefore, given K and C , the corresponding s_z is very easy to calculate. This is in general not the case as we have seen in equation (10). We have plotted the dependence of s on k and C in figure 1. As we can see, the value of s is always less than zero and never less than -1 , which is a reasonable behaviour.

Putting all these results together, the upper bound on correlations (entanglement) in equation (24) is now given by

$$\begin{aligned} E(\rho) \leq & \ln \left(2 \cosh \left[C - \frac{e^{-K} \sinh(2C)}{2(e^{-K} \cosh 2C + e^K \cosh 2K)} K \right] \right)^2 \\ & - \ln(2[e^{-K} \cosh 2C + e^K \cosh 2K]) \\ & + \frac{1}{Z} \{ (2C + K)e^{-(2C+K)} + Ke^{-K} + (-2C + K)e^{-(2C+K)} + (-3K)e^{3K} \} \\ & - \frac{1}{Z} \left\{ 2 \left[C - \frac{e^{-K} \sinh(2C)}{2(e^{-K} \cosh 2C + e^K \cosh 2K)} K \right] e^{-K} \sinh(2C) \right\}. \quad (32) \end{aligned}$$

We have plotted this bound in figure 2. We can see that it has a reasonable behaviour, in the sense that, for example, it increases with K as we expect correlations to increase with increasing interaction. Note that there is an increase in the value of the bound when $2K > C$. This is interesting when compared with the behaviour of entanglement. As mentioned earlier, entanglement also undergoes a transformation from a non-zero value to a zero value at this point [7]. We can also see some unreasonable behaviour from our approximation: the bound can be larger than 2, but the mutual information between two qubits can never exceed this amount. For some values of K and C , therefore, the bound becomes trivial (it is not wrong, strictly speaking, but it just becomes useless). Note that for $K = 0$ the bound also becomes zero, and hence there are no correlations between the spins. This is to be expected as K signifies the strength of the interaction and the absence of interaction means that the spins cannot become correlated in any way. For this case, our mean-field approximation becomes exact.

We can compare the bound to the true value of mutual information (which should be lower unless the mean-field approximation leads exactly to the closest product state!). This is just the

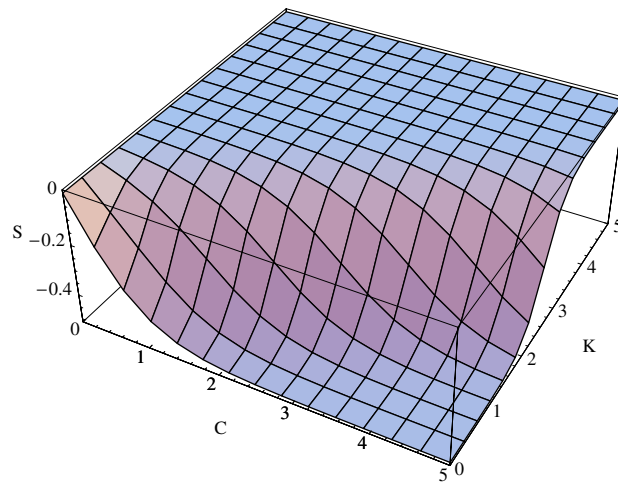


Figure 1. This figure shows the dependence of the mean field value of s on K and C . Note that there is a transition beyond the line $2K = C$, for which the value of magnetization becomes zero. This will be reflected in the behaviour of the bound on mutual information as seen in figure 2.

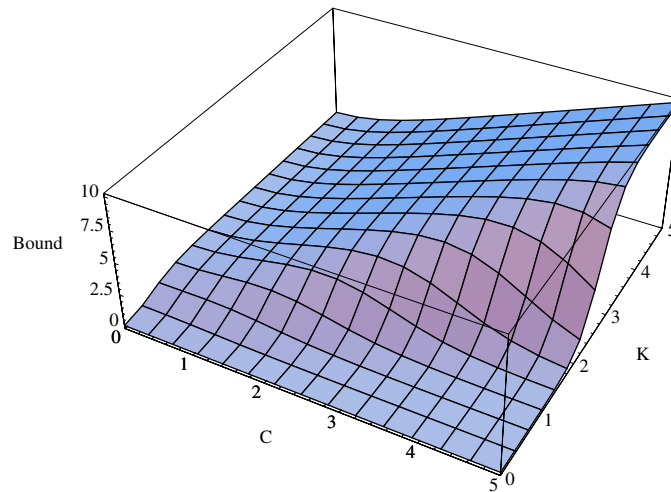


Figure 2. This figure shows the dependence of our bound on the amount of correlations for two Heisenberg spins as a function of K and C . Note the transition at $2K = C$ and the disappearance of correlations for $K = 0$.

difference between the sum of individual qubit entropies (which are equal to each other in this case) and the total two-qubit entropy, $I = 2S(\rho_1) - S(\rho)$. It is given by

$$\begin{aligned}
 I = & \frac{e^{-(2C+K)}}{Z} \ln \frac{e^{-(2C+K)}}{Z} + \frac{e^{-K}}{Z} \ln \frac{e^{-K}}{Z} + \frac{e^{-(-2C+K)}}{Z} \ln \frac{e^{-(-2C+K)}}{Z} + \frac{e^{3K}}{Z} \ln \frac{e^{3K}}{Z} \\
 & - 2 \left\{ \frac{e^{-K}/2 + e^{3K}/2 + e^{-(2C+K)}}{Z} \ln \left\{ \frac{e^{-K}/2 + e^{3K}/2 + e^{-(2C+K)}}{Z} \right\} \right. \\
 & \left. + \frac{e^{-K}/2 + e^{3K}/2 + e^{-(-2C+K)}}{Z} \ln \left\{ \frac{e^{-K}/2 + e^{3K}/2 + e^{-(-2C+K)}}{Z} \right\} \right\}. \quad (33)
 \end{aligned}$$

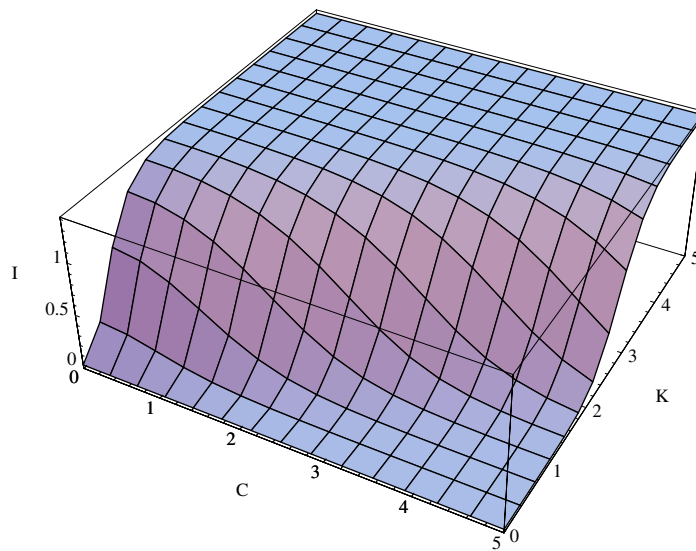


Figure 3. The exact dependence of mutual information for the two-spin Heisenberg model on the values of K and C . As noted in the text, there are no correlations in the absence of the interaction K .

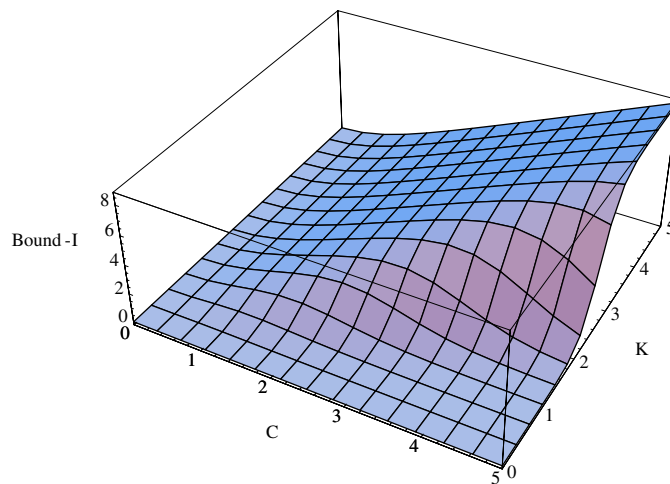


Figure 4. The difference between the bound and the exact value of I as a function of K and C .

This function is plotted in figure 3. Although the behaviour is different, the same transition occurs at $2K = C$.

We can see that our bound is always greater than this value (as it should be!). Figure 4 shows the difference between the bound on correlations and the actual mutual information. Note that for $K = 0$ and in the vicinity of this region the bound still gives exact results.

We are now in a position to apply our ideas to a much more complex model, whose features are still being investigated [19].

6. 1D Ising model in a transverse field

This model has been extensively used in many situations and has been analysed in various regimes [19]. The interesting feature of the Hamiltonian which makes it different from the ordinary classical Hamiltonian is that the interaction part of the Hamiltonian and the external field point in different mutually orthogonal directions. This makes the model more complex than if the two parts of the Hamiltonian were in the same direction (as in the original Ising model). One of the main consequences is that while there is never any entanglement present in the original Hamiltonian model, the one in the transverse field can exhibit entanglement [8].

The 1D Ising model in a transverse field is completely specified by the following Hamiltonian:

$$H = -\frac{J}{2} \sum_{i=1}^N \sigma_i^x \otimes \sigma_{i+1}^x - B \sum_{i=1}^N \sigma_i^z. \quad (34)$$

We first briefly summarize how to diagonalize this Hamiltonian [18]. The main tools are the Jordan–Wigner transformation, followed by a Fourier transform and finally followed by the Bogoliubov transform. What this achieves is the following: the initial spins, which are localized fermions, are subsequently converted into highly non-local fermions and then the delocalized fermionic Hamiltonian is easily diagonalized to find its spectrum. To simplify the mathematics even further at this point we will divide the Hamiltonian by $J/2$ and use as the only variable $\lambda = 2B/J$, so that

$$H = -\sum_{i=1}^N \sigma_i^x \otimes \sigma_{i+1}^x - \lambda \sum_{i=1}^N \sigma_i^z. \quad (35)$$

We will go back to the original Hamiltonian, recovering B and J at the end when we present results of our calculations. The spin operators in this expression satisfy anticommutation rules at any given site (just like fermions) but follow commutation rules at separate sites (again just like fermions). The non-local Jordan–Wigner transformation maps these operators into fully anticommuting spinless fermions defined by

$$a_l = \prod_{m < l} \sigma_m^z \frac{\sigma_l^x + i\sigma_l^y}{2} \quad (36)$$

such that

$$\{a_l^\dagger, a_m\} = \delta_{lm}, \quad \{a_l, a_m\} = 0. \quad (37)$$

In terms of operators a the above Hamiltonian becomes

$$H = \frac{1}{2} \sum_{l=-(N/2)+1}^{(N/2)-1} \{(a_{l+1}^\dagger a_l + a_l^\dagger a_{l+1}) + (a_l^\dagger a_{l+1}^\dagger + a_{l+1} a_l)\} - \lambda \sum_{l=-(N/2)+1}^{(N/2)} a_l^\dagger a_l. \quad (38)$$

We now introduce the Fourier transformed (fermionic) operators

$$d_k = \frac{1}{\sqrt{N}} \sum_{l=-(N/2)+1}^{(N/2)-1} a_l e^{-i(2\pi/N)kl}, \quad (39)$$

$-(N/2) + 1 \leq k \leq N/2$. Due to the fact that this transformation is unitary, the anticommutation relations remain true for the new d -operators. The Hamiltonian now takes an almost diagonal form,

$$H = \sum_{k=-(N/2)+1}^{N/2} \left(-\lambda + \cos \frac{2\pi k}{N} \right) d_k^\dagger d_k + \frac{i}{2} \sum_{k=-(N/2)+1}^{N/2} \sin \frac{2\pi k}{N} (d_k d_{-k} + d_k^\dagger d_{-k}^\dagger), \quad (40)$$

where an extra term, suppressed by $1/N$, should be present. This term clearly tends to zero as $N \rightarrow \infty$ and we can therefore safely omit it as all our results will refer to the thermodynamic limit.

A final unitary transformation is now necessary to cast the Hamiltonian into a manifestly diagonal form. This so-called Bogoliubov transformation can be expressed as

$$b_k^\dagger = u_k d_k^\dagger + i v_k d_{-k} b_k = u_k d_k - i v_k d_{-k}^\dagger, \quad (41)$$

where

$$u_k = \cos \theta_k / 2, \quad v_k = \sin \theta_k / 2$$

$$\text{for } \cos \theta_k = \left(-\lambda + \cos \left(\frac{2\pi}{N} \right) k \right) / \sqrt{\left(\lambda - \cos \frac{2\pi k}{N} \right)^2 + \sin^2 \frac{2\pi k}{N}}.$$

Again, due to unitarity of the Bogoliubov transformation the b -operators follow the usual anticommutation relations. Finally, the Hamiltonian takes the following diagonal form:

$$H = \sum_{k=-(N/2)+1}^{N/2} \tilde{\Lambda}_k b_k^\dagger b_k, \quad (42)$$

where

$$\tilde{\Lambda}_k \equiv \sqrt{\left(\lambda - \cos \frac{2\pi k}{N} \right)^2 + \sin^2 \frac{2\pi k}{N}}. \quad (43)$$

The thermodynamical limit is obtained by defining $\phi = 2\pi k/N$ and taking the $N \rightarrow \infty$ limit

$$H = \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \Lambda_\phi b_\phi^\dagger b_\phi, \quad (44)$$

with

$$\Lambda_\phi^2 = (\lambda - \cos \phi)^2 + \sin^2 \phi = K^2 + C^2 - 2KC \cos \phi. \quad (45)$$

We have in the last step reintroduced the K and the C parameter in order to recover the field and interaction dependence which will be important in our subsequent analysis. The exact partition function can be immediately calculated from here (this was originally done by Katsura [18]). In the large- N limit (which is what we are always interested in when it comes to computing thermodynamical quantities) we have

$$\ln Z = N \ln 2 + N \frac{1}{\pi} \int_0^\pi \ln \{ \cosh \sqrt{K^2 + C^2 - 2KC \cos \omega} \} d\omega. \quad (46)$$

We now need to construct a mean-field Hamiltonian. Let us try to approximate this Hamiltonian with the following one:

$$H_{MF} = \sum_l \left(-\frac{1}{2} s J \sigma_l^x - B \sigma_l^z \right). \quad (47)$$

This Hamiltonian is completely local and its eigenstates cannot be entangled (not even classically correlated). The parameter s is meant to approximate the effect of all other spins on the spin l . We will at the moment leave the value of s undetermined. The eigenvalues of $-\frac{1}{2} s J \sigma_l^x - m B \sigma_l^z$ are easily computed to be

$$\lambda_{\pm} = \pm \sqrt{B^2 + \frac{1}{4} s^2 J^2}. \quad (48)$$

The mean-field partition function is, therefore, given by

$$Z_{MF} = 2^N (\cosh \sqrt{C^2 + s^2 K^2})^N, \quad (49)$$

where, as before, $C = B/kT$ and $K = J/2kT$. The N th power again reflects the fact that there are N spins each with the same identical partition function. The free energy is in the mean-field theory now proportional to

$$\ln Z_{MF} = N \ln 2 + N \ln \{ \cosh \sqrt{C^2 + s^2 K^2} \}. \quad (50)$$

To complete the upper bound on thermal entanglement for the whole chain we need to estimate the average of the difference between the mean-field Hamiltonian and the true Ising Hamiltonian. The average of H is known from the partition function and it is [18]

$$\langle H \rangle_H = -NkT \frac{1}{\pi} \int_0^\pi \sqrt{K^2 + C^2 - 2KC \cos \omega} \tanh \sqrt{K^2 + C^2 - 2KC \cos \omega} d\omega. \quad (51)$$

The final quantity left to calculate is the average of the mean-field Hamiltonian which requires us to compute the averages of σ_z and σ_x . The average of the former is known and it is

$$\langle \sigma_z \rangle_H = Nm \frac{1}{\pi} \int_0^\pi \frac{(C - K \cos \omega) \tanh \sqrt{K^2 + C^2 - 2KC \cos \omega}}{\sqrt{K^2 + C^2 - 2KC \cos \omega}} d\omega. \quad (52)$$

The biggest problem is now the calculation of the average of the σ_x operator. This value is not known analytically unless $\beta \rightarrow \infty$. So, instead of calculating this value exactly, we will assume that $\langle \sigma_x \rangle = s$.

Putting all the results together we obtain the following bound on the amount on entanglement:

$$\begin{aligned} E(\rho) \leq N \Bigg\{ & \ln \{ \cosh \sqrt{C^2 + s^2 K^2} \} - \frac{1}{\pi} \int_0^\pi \ln \{ \cosh \sqrt{K^2 + C^2 - 2KC \cos \omega} \} d\omega \\ & + \frac{1}{\pi} \int_0^\pi \sqrt{K^2 + C^2 - 2KC \cos \omega} \tanh \sqrt{K^2 + C^2 - 2KC \cos \omega} d\omega - Ks^2 \\ & - C \frac{1}{\pi} \int_0^\pi \frac{(C - K \cos \omega) \tanh \sqrt{K^2 + C^2 - 2KC \cos \omega}}{\sqrt{K^2 + C^2 - 2KC \cos \omega}} d\omega \Bigg\}. \end{aligned} \quad (53)$$

We now turn our attention to calculating the value of s which is necessary to use the above bound. Again, we cannot calculate the real value of s in the state ρ , but need to simplify and assume that $s = \langle \sigma_x \rangle_{H_{MF}}$. This means that we only need to calculate the average of σ_x in the mean field and this is a simple task. For this we need the eigenvalues and eigenvectors of the mean-field Hamiltonian. The former have already been used, and the latter are (in general) given by

$$|\psi_+\rangle = a|0\rangle + b|1\rangle, \quad (54)$$

$$|\psi_-\rangle = b|0\rangle - a|1\rangle \quad (55)$$

(a and b are real), where it can be calculated that

$$ab = -\frac{K(C + \sqrt{C^2 + s^2 K^2})}{K^2 + (C + \sqrt{C^2 + s^2 K^2})^2} \quad (56)$$

(it turns out that we will ever need only the value of the product of a and b and not their individual values). The average value of the Pauli x operator is now:

$$s = \langle \sigma_x \rangle_{H_{MF}} = \frac{2K(C + \sqrt{C^2 + s^2 K^2})}{K^2 + (C + \sqrt{C^2 + s^2 K^2})^2} \tanh \sqrt{C^2 + s^2 K^2} \quad (57)$$

and this therefore presents the equation from which we should determine the value of s . The algorithm for computing the upper bound on the total amount of entanglement is now the following:

- Given the values of K and C , first compute the corresponding value of $s = s(K, C)$;
- Then compute the value of the upper bound for the same three values of K , C and s .

We can, of course, always handle this problem numerically and some numerical results will indeed be presented. We will first discuss the estimation of the critical temperature beyond which we do not have the solution for the average magnetization in the mean-field approximation. Even though this is impossible to do analytically (we have a transcendental equation), we can always look at some special cases. For example, when the external field vanishes, $C = 0$, we have that

$$\tanh Ks = \frac{1 + s^2}{2}. \quad (58)$$

The solutions of this equation exist only if $K > K_c$ which implies that $T < J/2kK_c$, k being the Boltzmann constant. In this case, we can numerically estimate that $K_c \approx 1.37$. Note that if, on the other hand, $K = 0$, then it follows immediately that $s = 0$. It is also not so difficult to obtain other critical regions. For example, for $C = 1$, all values of $K \geq 8$ yield the value of s outside the acceptable region (which is between -1 and 1). In general, therefore, it is first important to investigate the domain of validity of the approximation before we can use the bound on correlations.

Before we analyse the general values of the interaction, external field and temperature, let us first investigate a few special cases which can be addressed immediately and analytically. First of all, as K tends to zero (while C is kept finite), the value of the upper bound tends to zero.

Therefore, there is no entanglement present here. This is expected as the small- K limit implies that the external field dominates the interaction part and then the eigenstates become product states of all spins pointing in the z direction which is a completely disentangled state (this is why the average magnetization in the x direction, s , tends to zero as it is equally likely to point in the positive and negative directions).

The opposite limit is when K becomes large (while C is still kept finite). Then, as the interaction dominates the external field, the state of the system approaches the product of spins all aligned and pointing in the x direction (the ground state is when all the spins assume the same eigenvalue of x , the first excited states are the ones where one of the spins has an x value opposite to the rest, and so on). Therefore, we should expect no entanglement in this case, although it may seem surprising that a strong interaction ultimately does not produce entangled states. From the bound we obtain

$$\frac{E(\rho)}{N} \leq K(s - s^2). \quad (59)$$

The mean-field theory also implies that $s \rightarrow 1$, and so entanglement indeed disappears as the bound tends to zero.

The third special case we analyse is when $C = K \rightarrow \infty$. There are two different physical situations when this limit is reached. One is to keep the temperature constant and increase the external field and the interaction strength at the same rate. The other is to keep B and J fixed and decrease the temperature to zero. From the mean-field approximation we can obtain the value of $s \approx 0.75$. This then gives us the bound on entanglement as

$$\frac{E}{N} \leq \left\{ \frac{11}{16} - \frac{1}{\pi} \int_0^\pi \sqrt{1 - \cos \omega} d\omega \right\} \approx 0.2K. \quad (60)$$

The regime $T = 0$ has been extensively studied [19] and, as we discussed before, there is a quantum critical point of B at which some thermodynamic potentials (such as the free energy) become non-analytic. At $T = 0$, the critical region is when $B < J/2$ [19] (in other words, this is the $C < K$ region, but both in the large limit). This behaviour is confirmed by our calculation as will be seen when we present plots of the bound. Note, however, that the upper bound on information per spin grows linearly with K . Since the mutual information per spin cannot be larger than the entropy of the spin, which has its maximum at $\ln 2$, this means that the bound becomes useless for $K > 5$. This number has been calculated only approximately and in the limit of large K . Nevertheless, there will still be a cut-off of this kind beyond which our approximation is no longer useful (although it is still, of course, valid, but only trivially).

In the case of the Heisenberg model with two qubits we compared the bound to the exact value of the mutual information. Can we do the same here? The answer is that, in general, this is not possible. Some special cases can be addressed (such as the zero temperature, ground-state entanglement and entropies as in [15]), but for any generic values of C , K , T it appears very difficult to obtain the single-spin density matrix. In particular, while we are able to compute the average value of σ_z , there is no way of computing the x and y components necessary to fully infer the state. This therefore prevents us from calculating the total mutual information which would be equal to $I = NS(\rho_1) - S(\rho)$. This is why the method presented here may be useful in estimating correlations. Note that the total entropy $S(\rho)$, on the other hand, can be computed, as we know the spectrum exactly.

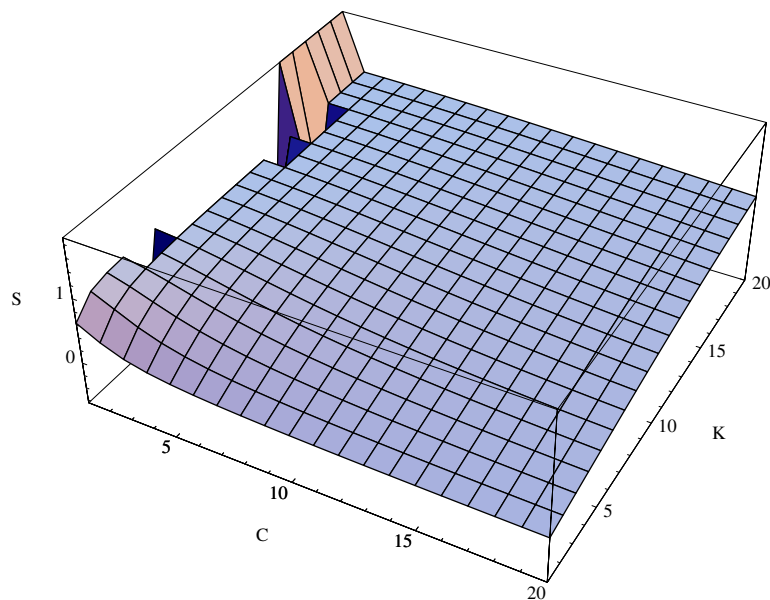


Figure 5. The dependence of our mean-field magnetization s on the parameters K and C .

Now we will plot the value of the upper bound for the Ising model in a transverse field for a range of values of K and C . This is exactly what we did in the case of two Heisenberg interacting spins. We will first reproduce the plot of the mean-field value of s (which will be a transcendental equation in this case, and hence not analytically solvable) and then use this value to plot the upper bound on correlations. The numerical results here will also show the region where the approximation holds and where it definitely fails.

Figure 5 shows the dependence of the mean-field magnetization on the external field and the coupling. One region of failure of the mean-field approximation for this model can immediately be seen from the plot. Note that for $C = 1$ we have that there are some values of s which are higher than one (in general, we have that $|s| \leq 1$). This is a sufficient condition for failure, but not necessary. There are other regions where the approximation fails, but they will not be discussed here.

With this in mind, we can now go ahead and plot the upper bound using the results for the magnetization from figure 5. Figure 6 displays the plot of the upper bound. The first thing that strikes is the existence of two different regions, separated by the boundary where $K = C$. This, very interestingly, coincides with the existence of the critical region, $K > C$, known as the quantum criticality as introduced by Sachdev [19]. We have already remarked that the quantum criticality is only manifested at zero temperature, and by varying the strength of the external field. In our case, this coincides with the domain when $K, C \rightarrow \infty$. In our bound, the separation between regions exists, on the other hand, for any value of K and C . There is no discontinuity here between the finite-temperature region and the $T = 0$ region. It is not clear to us if this finding has any more general significance regarding the behaviour of the solid. Note also that there is a non-smooth behaviour for small values of C , just where the value of s from the mean-field theory also fails to be in the region $\{-1, 1\}$. Intuitively, we expect the approximation to fail here as we are in the region where the external field is dominated by the interaction, and the mean-field approximation neglects the interaction completely.

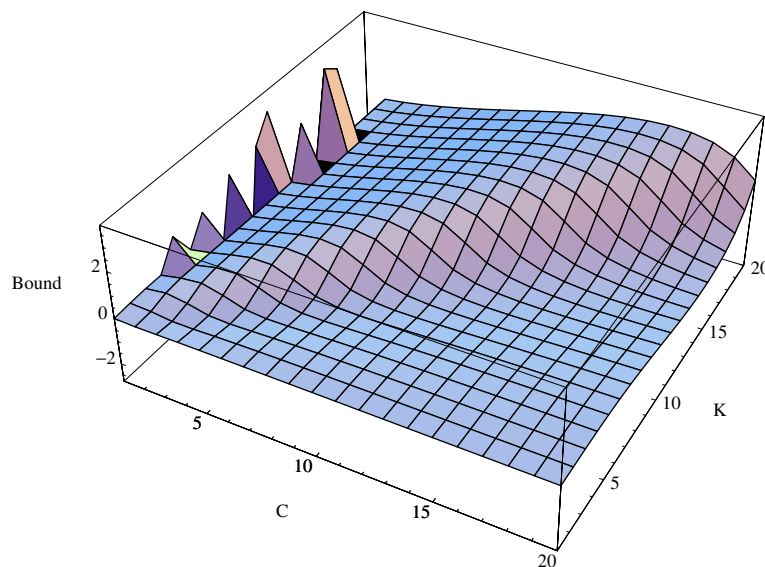


Figure 6. The dependence of the correlation bound on the parameters K and C . Note that the region for which $K > C$ shows an increase in the bound. This coincides with the notion of the quantum phase transition.

Having obtained the above results, how much should we trust our method? In other words, what is the domain of validity of the mean-field approximation? First of all, we can see when the method obviously fails. This is, as we mentioned above, when the value of the magnitude (absolute value) of s becomes greater than 1. Also, the method fails when the bound on correlations per spin exceeds the maximum value of 1. We have already commented when this happens in our model. There is, however, a more general way of assessing the validity of the approximation. We will only present a sketch of this argument here, and a much more general analysis can be found in any book on advanced statistical mechanics (e.g. [16]).

The usual way of deriving the limitations of the mean-field approximation is to look at the regime where fluctuations due to interactions become large. This is when we expect the mean field to fail since the mean field neglects those interactions. How can this regime be determined more precisely? We know that the susceptibility is given by the following expressions:

$$\chi = \frac{\partial \bar{M}}{\partial B} = \frac{\bar{M}^2 - (\bar{M})^2}{kT} = \frac{\Delta \bar{M}^2}{kT}, \quad (61)$$

where \bar{M} is the average magnetization. We can recast the second equality to obtain:

$$\frac{\Delta \bar{M}^2}{(\bar{M})^2} = \frac{kT\chi}{(\bar{M})^2}. \quad (62)$$

For fluctuations to be small we need to have that

$$kT\chi \ll (\bar{M})^2. \quad (63)$$

More detailed calculations of $(\bar{M})^2$ [16] suggest that the dimensionality of the system would have to be greater than 4 in order for this to be correct. This is intuitively satisfactory, as higher

dimensions imply that each spin has more neighbours and therefore we expect to obtain a better mean-field average. In other words, this means that the overall state displays a low degree of correlations. Indeed, for the mean field and the exact susceptibility to be approximately equal, i.e.

$$\chi_{MF} - \chi \approx 0, \quad (64)$$

we have

$$kT \frac{\partial^2 I}{\partial B^2} \approx \frac{\partial^2 \langle H - H_{MF} \rangle_H}{\partial B^2}. \quad (65)$$

Thus the, smaller the mutual information I , the better the mean-field approximation. The conclusion of the ‘back-of-an-envelope’ type of analysis is that we should not expect the 1D mean-field approximation to be very accurate here. Nevertheless, the results presented in this section indicate that there is a general agreement with other results obtained for this model. Generalizations of our method to higher dimensions would certainly be most welcome.

We would now like to discuss another question of very general importance. So far, we have been careful to point out that our bound has been limiting the amount of total correlations, and thus entanglement, but we have not tried to discriminate between the quantum and the classical contribution to correlations. Recently, however, we have seen claims that the effects of entanglement on the macroscopic properties are genuinely different from the effects of classical correlations [1]. But, how can we be sure that entanglement is possible in a solid and that its effects cannot be reproduced by the ordinary, classical correlations?

7. Classical versus quantum correlations

We have so far been discussing the effect of correlations as quantified by the mutual information on the macroscopic quantities for some simple (1D) spin models. Of course, in a real solid, there is usually a large number of degrees of freedom and here we are approximating them only with spin-half systems. So, how to ensure that we have really identified effects of entanglement as opposed to some kind of interaction between these large multitude of neglected degrees of freedom? Is it possible to reproduce the effect of entanglement by allowing more degrees of freedom? The answer is ‘yes’, and hence we have to be very careful under those circumstances if we are to identify something as a clear effect of entanglement. We will first illustrate this with a very simple example, and then discuss a more general model, which is extensively used in statistical mechanics, field theory and condensed matter physics.

Suppose that we have two correlated qubits. The maximum value of entanglement is $\ln 2$, however the mutual information can be as large as $2 \ln 2$. Our understanding of this difference is that the mutual information represents the total correlations and is therefore the sum of quantum and classical correlations (whatever they are defined to be, see [20] for one possible entropic definition). This would suggest that in a maximally entangled state of two qubits we have $\ln 2$ of classical correlations (for two qubits we cannot have more than this amount of classical correlations) and $\ln 2$ of entanglement. So, having two qubits and knowing that $I = 2 \ln 2$ immediately implied a maximal unit of entanglement. However, suppose that these two qubits were really two 4-level systems. Then classical correlation would be by itself as high as $2 \ln 2$.

In such a case, the mutual information of $2 \ln 2$ would not necessarily imply the existence of any entanglement. Therefore, the actual dimensionality of our constituents is very important.

It is well known that d -dimensional quantum statistical models are isomorphic to $(d + 1)$ -dimensional problems in classical statistical mechanics. Let us illustrate this with a very simple example of a quantum mechanical two-level system—a qubit. The question we would like to ask is: if there is entanglement in the d -dimensional quantum system how is that reflected in the $(d + 1)$ -dimensional classical system?

Let us review how this correspondence works. Suppose we have a quantum system with the Hamiltonian H . Since this is a single system, its dimension $d = 0$. We will now show how to correspond this to a $(d = 1)$ -dimensional classical system. The partition function is given by

$$Z = \text{tr} e^{-\beta H} = \sum_i \langle \psi_i | e^{-\beta H} | \psi_i \rangle, \quad (66)$$

where $\{|\psi_i\rangle\}_1^N$ is some orthonormal basis. Invoking the completeness relations $\sum |\psi_i\rangle\langle\psi_i| = 1$, this can be written as

$$\begin{aligned} Z &= \lim_{N \rightarrow \infty} \sum_i \left\langle \psi_i \left| \left(1 - \frac{\beta H}{N}\right)^N \right| \psi_i \right\rangle = \lim_{N \rightarrow \infty} \sum_{i_1, i_2, \dots, i_N} \left\langle \psi_{i_1} \left| \left(1 - \frac{\beta H}{N}\right) \right| \psi_{i_2} \right\rangle \\ &\quad \times \left\langle \psi_{i_2} \left| \left(1 - \frac{\beta H}{N}\right) \right| \psi_{i_3} \right\rangle \times \dots \times \left\langle \psi_{i_N} \left| \left(1 - \frac{\beta H}{N}\right) \right| \psi_{i_1} \right\rangle. \end{aligned}$$

This is still a quantum mechanical expression and now we will translate it into a ‘classical Hamiltonian’. Suppose we require that

$$\left\langle i \left| \left(1 - \frac{\beta H}{N}\right) \right| j \right\rangle = A \exp(Bij + Ci + Dj), \quad (67)$$

where i, j are numbers taking values ± 1 and represent the two values of the spin (note that it is now more convenient for notational purposes to label the eigenstates as $|\pm 1\rangle$). The values of A, B, C and D can be inferred from this equality. Using the right-hand side of the equality (the classical Hamiltonian) we can write the original partition function as

$$Z = \lim_{N \rightarrow \infty} A^N \sum_i \exp(Bu_i u_{i+1} + hu_i), \quad (68)$$

where $h = C + D$ and, to make the notation closer to the classical Ising model, we have used u_i instead of i . Note that this is now the same as a classical 1D Ising-like model with nearest-neighbour interactions. In fact, this method of equating the quantum evolution in d dimensions to a classical statistical problem in $d + 1$ dimensions has been extensively exploited (see [22]). There is a calculational advantage here since it is easier to treat exponentials of numbers (on the right-hand side) than exponentials of operators (which are on the left-hand side), but here we are not interested in this aspect.

Suppose that we have a qubit whose Hamiltonian is given by

$$H = \begin{pmatrix} E & -\Delta \\ -\Delta & -E \end{pmatrix},$$

where E and Δ are just some real numbers. The solutions of equation (67) are given by

$$A = \left(\frac{\beta \Delta}{N} \right)^{1/2} \left(1 - \frac{\beta^2 E^2}{N^2} \right)^{1/4}, \quad (69)$$

$$B = \frac{1}{4} \ln \left(\frac{N^2 - \beta^2 E^2}{\beta^2 \Delta^2} \right), \quad (70)$$

$$h = \frac{1}{2} \ln \left(\frac{N - \beta E}{N + \beta E} \right). \quad (71)$$

We are now in a position to address the question at the beginning of this section: if $\rho = e^{-\beta H}/Z$ is an entangled state, how is that entanglement reflected in the classical analogue?

The above treatment is suitable for a single-spin system. When we have two spins, then we need more variables in the classical model. One way of dealing with this is the following: take a classical chain to represent each of the qubits. To simulate the interaction Hamiltonian between the qubits creating entanglement (correlations in general), we need the two chains to interact. This is a straightforward application of the above formalism. Therefore, in order to claim that some thermodynamical property is a consequence of two-qubit entanglement, we need to make sure that we indeed have two qubits (and not a classical chain of bits simulating that qubit). What happens if we have N qubits interacting? Then we need a 2D classical square lattice of interacting spins to simulate this. A good instance of this is the 2D classical Ising model. This, in fact, is the reason behind the fact that the 1D partition function of a transverse Ising model resembles the partition function of Onsager for the 2D Ising model [21]. Therefore, it is not trivial to show that entanglement is responsible for some macroscopic effects, since by enlarging our system, classical correlations can also sometimes be used to derive the same conclusion.

At the end, we would like to point out that the above method of making the quantum–classical correspondence is by no means the only one. Another way of representing two interacting qubits is to make the coefficient B spin-dependent. Then we can write

$$\left\langle i \left| \left(1 - \frac{\beta H}{N} \right) \right| j \right\rangle = A \exp(B_{ij} i j + C i + D j), \quad (72)$$

where B_{ij} are the spin-dependent coefficients. Either way, we see that entanglement in one dimension can always be (at least in principle) interpreted as just classical correlations in a higher dimension. The significance that this quantum–classical correspondence may have for our purposes, if any, is ultimately completely unclear. What is clear, however, is that we have to be very careful to interpret something as an effect of entanglement unless we are sure that the extra dimensions do not contribute the extra (purely classical) correlations. One way to ensure that entanglement is present is to test some form of Bell's inequalities, between two spatially separated parts of the solid, thereby ruling out any local classical correlations, but it is not entirely clear how to do this and we leave this issue for future research.

8. Conclusions

In this paper we attempted to derive an upper bound on the amount of correlations in a solid. Our method can be linked to one way of deriving the Bogoliubov bound. We have applied it to two

scenarios: two qubits with Heisenberg interaction, which was just used to illustrate our method, and a chain of qubits with Ising interaction but placed in an external transverse field. We have also discussed several limitations of this method. Although the upper bound presented here can tell us a great deal about total correlations, and therefore also about the entanglement bound, in order to gain a better understanding it would be advantageous to find similar lower bounds. For example, the sum of all bipartite entanglements per qubit is one such bound and it is relatively easy to compute. In fact, for the Ising model in a transverse field (and at zero temperature) we have the results to compute this [7, 14]. It would be important, therefore, to try to derive a tight lower bound on entanglement (and correlations in general), and this we believe will be a very useful direction for future research. Another problem is to consider the spin of particles involved [23]. This will add the particle statistics into our picture and, as is well known, can affect the amount of entanglement, as well as being able to convert entanglement for the internal degrees of freedom to the spatial (external) degrees of freedom [23]. Although some methods have been developed for quantifying entanglement under such circumstances, the relationship between ‘internal’ and ‘external’ entanglement is still not properly understood and the problem would be well beyond the scope of the current investigations.

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