Cluster Entanglement Mean Field inspired approach to Criticality in Classical Systems

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We propose an entanglement mean field theory inspired approach for dealing with interacting classical many-body systems. It involves a coarse-graining technique that terminates a step before the mean field theory: While mean field theory deals with only single-body physical parameters, the entanglement mean field theory deals with single- as well as two-body ones. We improve the theory to a cluster entanglement mean field, that deals with a fundamental unit of the lattice of the many-body system. We apply these methods to interacting Ising spin systems in several lattice geometries and dimensions, and show that the predictions of the onset of criticality of these models are much better in the proposed theories as compared to the corresponding ones in mean field theories.

I. INTRODUCTION AND MAIN RESULTS

The search for bridges between many-body physics and quantum information has been very fruitful, and has led to many important discoveries and insights [1, 2]. On the one hand, quantum information concepts have been used to provide further tools to a many-body physicist, while on the other, realizable many-body physics systems ranging from quantum optics systems to ion traps are being tried as potential substrates for quantum information processing tasks.

It is rarely possible to treat an interacting many-body system exactly, and hence it is important to obtain approximate methods to deal with them. The mean field theory (MFT) [3–5], introduced by P. Weiss in 1907, is a very useful tool available to many-body physics to examine such systems, for both classical and quantum interacting many-body systems, with a low computational cost.

Main thesis. We propose that parallel to, but clearly different from, the MF class of theories [3], there exists an entanglement mean field class of theories to treat interacting classical many-body systems, that deals with one-body and two-body physical parameters in its self-consistency equations.

The mean field class of theories are an ultimate form of coarse-graining of the many-body system, in that it reduces the interacting many-body Hamiltonian to single body terms, and deals with single-body physical parameters in its self-consistency equations [3]. In contrast, the entanglement mean field class of theories proposes to stop a step before in the coarse-graining process, and reduces the parent Hamiltonian to a finite number of two-body terms, and deals with single- as well as two-body terms in its self-consistency equations.

The entanglement mean field class of theories provides us with a tool to go beyond the mean field class, and yet remain in the low-cost bracket. We believe that the formalism will be useful in investigation and control of many-body systems in several areas including condensed matter, ultra-cold gases, and quantum information.

An interesting improvement of the mean field approach is the cluster mean field theory (CMFT) [6], where one reduces the many-body system to a fundamental unit ("cluster") of the many-body lattice, while still retaining footprints of the many-body parent as an undetermined parameter, although this undetermined parameter is still (like in MFT) a one-site physical quantity (like, magnetization) of the many-body parent, and it is determined by the self-consistency relation (CMF equation) equating the parameter to the same one-site quantity obtained from the cluster. We stress here that the self-consistency relations in *both* MFT and CMFT are are based on *one*site physical quantities, in particular, on magnetization.

To treat critical phenomena in interacting classical spin models inspired by entanglement mean field theory (EMFT), proposed for quantum systems in Ref. [7], one reduces the many-body classical system to a two-body one while retaining imprints of the many-body parent as an undetermined parameter. In contrast to MFT, in EMFT, the undetermined parameter depends on a twosite physical quantity (like, two-point correlation) of the many-body parent. This parameter is then determined by the self-consistency relation (EMFT equation) equating, e.g. the two-point correlation of the many-body parent with that of the EMFT-reduced two-body system. Note that there is certainly no quantum entanglement [8] generated by applying the EMFT to classical spin systems.

We stress here that that the entanglement mean field theory is different from the cluster mean field approach. While the latter uses single-site physical parameters in its self-consistency equation, the former uses two-site ones. EMFT is also different from other useful techniques to deal with many-body systems, like the renormalization group approaches [9], with the latter using block decimation techniques on the whole lattice. These differences, both operational and result-wise, will be further underlined in Sec. II.

In this paper, we also present a further improvement of EMFT to a "cluster EMFT" (CEMFT) that reduces the many-body system to a fundamental unit of the many-body lattice, while retaining impressions of the original many-body system as undetermined parameters. In contrast to CMFT, in CEMFT, the undetermined parameters depend *both* on one-site and two-site physical quantities (e.g., on magnetization and two-site correlation) of the many-body parent. These parameters are then de-

termined via *coupled* self-consistency equations (CEMFT equations) equating e.g. the magnetization of the original many-body system with that of the (CEMFT-reduced) cluster, and the two-point correlation of the many-body parent with that of the cluster.

Apart from CMFT, there are several other interesting generalizations of the mean field theory in the literature, including the Bethe-Peierls-Weiss approximation [10], the Onsager reaction field theory [11], the diagrammatic expansion method [12] the self-consistent correlated field theory [13], the screened magnetic field theory [14], and the correlated cluster mean field theory [15], to mention a few (see also [16]). Improvements of the entanglement mean field theory in these directions are also possible, and will be pursued later. Meanwhile, let us note here that all the above exciting examples, in the MF class of theories, deal with single-body physical parameters in the respective self-consistency equations. In contrast, the EMF class of theories deal with single- as well as two-body physical parameters in the EMFT class self-consistency equations.

MFT vs. EMFT. Solving for magnetization and correlation functions from the EMFT and CEMFT equations leads to the prediction of critical phenomena in the spin models. We apply the EMF and CEMF theories to the nearest-neighbor Ising model in one, two (hexagonal, square, and triangular), and three (cubic), dimensional lattices. The results are given in Table 1. In all the cases considered, in the different dimensions and geometries, EMFT gives better predictions over MFT, and CEMFT is better than CMFT. (Actually, EMFT is already better than CMFT in all the cases considered.) In the best case, EMFT is better than MFT by 68% and CEMFT is better than CMFT by 85%, happening respectively for the hexagonal and square lattice systems. In the worst case, EMFT is better than MFT by 42%, and CEMFT is better than CMFT by 8%, happening respectively for the triangular and cubic lattice systems.

II. EMFT FOR CLASSICAL MODELS

Before presenting the entanglement mean field theory inspired approach to classical spin models, let us briefly describe the mean field theory for such systems. Consider the nearest neighbor (classical) Ising model

$$H = -J \sum_{\langle \vec{i}\vec{j} \rangle} \sigma_{\vec{i}} \sigma_{\vec{j}} \tag{1}$$

which represents a system of interacting (classical) spin-1/2 particles (Ising spins) on a *d*-dimensional lattice of an arbitrary fixed geometry. The coupling strength J is positive, and $\sigma_{\vec{i}} = \pm 1$ represents the value of the Ising spin at the site \vec{i} . $\langle \vec{ij} \rangle$ indicates that the corresponding sum runs over nearest neighbor lattice sites only.

The mean field theory consists in assuming that a particular spin, say at $\vec{i_0}$, is special, and replacing all other spin operators by their mean values. Denoting the mean values of the spin operator $\sigma_{\vec{i}}$ at the site \vec{i} by m (average magnetization), leads to an MFT Hamiltonian [3], which we denote as H_{MFT} . One then solves the self-consistency equations (mean field equations)

$$m = \sum_{\mathcal{CF}(\mathcal{I})} \sigma \rho_{MFT}^{\beta}, \qquad (2)$$

for m. Here ρ_{MFT}^{β} is the mean field canonical equilibrium state $\exp(-\beta H_{MFT})/Z_{MFT}$, $Z_{MFT} = \sum_{\mathcal{CF}(\mathcal{I})} \exp(-\beta H_{MFT})$) is the MF partition function, $\beta = \frac{1}{k_B T}$, with T denoting temperature on the absolute scale, and k_B the Boltzmann constant. Here, and in the rest of the paper, $\mathcal{CF}(\mathcal{I})$ will denote all Ising configurations of all the spins involved in that particular case. In the MF equation as well as in the MF partition function, there is just a single spin left, and $\mathcal{CF}(\mathcal{I})$ denotes the set of the two possibilities thereof. Substituting m in H_{MFT} and ρ_{MFT}^{β} , one can find the single-body physical properties of the system in the mean field limit.



FIG. 1: (Color online) MF vs. EMF class of theories. In MFT, a "magnifying glass" is put on a single particle of the many-body interacting system, and it leads to a self-consistency relation involving single-particle parameters. A different magnifying glass is employed in EMFT, which focusses attention on *two* particles, and leads to a selfconsistency relation involving *two-particle physical parameters*. Parallely, in CMFT, a fundamental unit (cluster) is chosen from the lattice which then is used to write selfconsistency equations, again involving only single-site parameters. In CEMFT, the same cluster is used, but the selfconsistency equations involve both one-site and two-site physical parameters.

The entanglement mean field theory begins by noting that the square of an Ising spin random variable is unity. The two-body interaction Hamiltonian that we are dealing with, can be thought of an N-body interaction Hamiltonian (N being the total number of Ising spins in the

system), in each term of which, all but two random variables are constant (= unity). Let us call it a unit random variable. Since the square of any Ising random variable is unity, we can replace a unit random variable on a site that is neighboring the nontrivial interacting spins of an interaction term, by the square the Ising random variable at that site, for all the interaction terms in the Hamiltonian. Therefore, the term $\sigma_{k-1,l}\sigma_{k,l}$ in a Hamiltonian on a two-dimensional square lattice can be replaced by $\sigma_{k-1,l}\sigma_{k,l}\sigma_{k+1,l}\sigma_{k+1,l}$. The latter can be re-written as AB, with $A = \sigma_{k,l}\sigma_{k+1,l}$, and $B = \sigma_{k-1,l}\sigma_{k+1,l}$. Let us call this Hamiltonian as H_{EMFT}^{inter} . For a given interaction term, let us call the site at which the replacement of the unit random variable by the square of the Ising random variable is done as the dummy site for that interaction term. Given an interaction term, there can be several nearby sites that can act as the dummy site for that term. So in the case of the term $\sigma_{k-1,l}\sigma_{k,l}$, (k+1,l)is used as the dummy site. We then assume that a certain *pair* of two neighboring spins are "special". (See Fig. 1.) Consider a *d*-dimensional lattice with coordination number ν_{co} . There will be $2(\nu_{co}-1)$ terms in the Hamiltonian H_{EMFT}^{inter} , that will have the special pair, along with two more Ising spins in two lattice sites (one of which, viz. the dummy site, is different from the special pair sites). In such a lattice, any one spin in the special pair is connected (via interactions in H) to $\nu_{co} - 1$ spins. Let this number $(\nu_{co} - 1)$ be denoted by ν_E , and be called the EMFT coordination number. We now replace the nonspecial two-spin interactions (with nearby spins) in all the interaction terms in H_{EMFT}^{inter} by a constant multiple of their mean values C. Physically, the mean value Crepresents the nearest neighbor correlation in the corresponding lattice. Since every interaction in H connecting to the special pair actually connects to one spin in the pair, the non-special two-spin interactions in each term in H_{EMFT}^{inter} is replaced by $\frac{1}{2}C$. The EMFT-reduced Hamiltonian, for the nearest neighbor Ising model on a d-dimensional lattice with EMFT coordination number ν_E , will therefore be

$$\mathcal{H}_{EMFT} = -\frac{1}{2} J \nu_E C \sigma_{\vec{i}} \sigma_{\vec{j}} \tag{3}$$

where we have ignored the terms in the Hamiltonian which will not contribute to the EMFT equations below, and where we have assumed that the neighboring lattice sites \vec{i} and \vec{j} are special. The self-consistency equation (EMFT equation) is

$$C = \sum_{\mathcal{CF}(\mathcal{I})} \sigma_{\vec{i}} \sigma_{\vec{j}} \varrho_{EMFT}^{\beta}, \qquad (4)$$

for a system at temperature T. Here ρ_{EMFT}^{β} is the entanglement mean field canonical equilibrium state $\exp(-\beta H_{EMFT})/Z_{EMFT}$, $Z_{EMFT} = \sum_{\mathcal{CF}(\mathcal{I})} \exp(-\beta H_{EMFT})$ is the EMF partition function. The EMFT equation is to be solved for C for obtaining the two-particle physical properties of H in the EMFT limit. In a typical situation, there is a finite temperature T_c , the critical temperature, that depends on the lattice geometry and dimension, above which the EMFT equation provides a nontrivial (i.e. nonzero) solution.

The values of the critical temperatures have been obtained for the interacting Ising systems in different dimensions and geometries, and are given in Table 1. The predictions of the EMF theory are always better than the corresponding ones from MFT in the cases considered, and almost always more than 50 percent better, and for the hexagonal (honeycomb) lattice in two dimesnions, EMFT is 68% better than MFT. See Table 1 for further details.

In the entanglement mean field theory, the nature of the interactions propagating in the lattice geometry, enters the predictions through the the existence of an interaction term $(\sigma_{\vec{i}}\sigma_{\vec{j}})$ and a two-site physical parameter (the mean correlation C) in the EMFT Hamiltonian H_{EMFT} , and their interplay in the self-consistency equation (EMFT equation). These features are absent in MFT, where the MFT Hamiltonian contains a single Ising random variable and a single-site physical parameter. Moreover, an EMFT coordination number enters the stage in EMFT, while it is the coordination number in MFT. These differences lead to the better memory of the EMFT of its many-body parent, and a consequent better performance of the EMFT over MFT.

Note that the EMFT approach is different from the cluster MFT [6] as there the fundamental unit changes with the lattice geometry and dimension, while here we always work with two special spins regardless of the lattice geometry. More importantly, the cluster MFT still (i.e., as in MFT) uses single-site properties to construct the self-consistency equations, while in EMFT, we use two-site properties to do the same. Additionally, both MFT and CMFT leads to effective Hamiltonians consisting of either a single random varible or a sum over single random variables, while in EMFT, we deal with effective Hamiltonians that retain interaction terms involving two random variables. These are some of the operational differences. Result-wise, a glance at Table 1 reveals that the predictions, for the critical temperatures of the different models, of EMFT and CMFT, are very different. Indeed, in all the cases considered, EMFT performs better than CMFT, with the prediction in the case of the threedimensional cubic lattice being 49% better. It is possible to obtain a generalization of the EMFT approach, towards a "cluster EMFT", for a better consideration of the lattice geometry, and we do so in the succeeding section.

The EMF approach is also different from the other techniques to handle many-body models. In particular, it is unlike the renormalization group approach [9], where block decimation techniques are used on the whole lattice, and free energy of the decimated lattice is equated to that of the original. Result-wise, application of the renormalization group to, e.g. the nearest neighbor Ising model on the square lattice predicts a critical temperature (in units of k_BT/J) at 2.55 [4]. The EMFT prediction is 3. The CEMFT prediction (considered below) is 2.08, with the exact value being 2.27 [17]

A similar formalism as above works (for both EMFT and cluster EMFT), with suitable modifications, for quantum spins, higher discrete spins, continuous spins, more complex lattices and interactions, etc. Also, both the mean field theory as well as the EMFT has been described for the ferromagnetic cases. The antiferromagnetic case requires some modifications in the mean field theory, and correspondingly some changes in the EMFT (and CEMFT). These will not be discussed in this paper.

III. CLUSTER EMFT FOR CLASSICAL MODELS

As has been noted before, the interactions of the manybody parent propagating in the lattice, are taken care of in the entanglement mean field theory, by the EMFT coordination number, and the interplay of the mean correlation C and the interaction term in H_{EMFT} in the selfconsistency equation. We have seen that this gives a better consideration to the interactions in the parent Hamiltonian than that in MFT. Towards improving our approximations, we now include the lattice structure along with interactions between spin variables. We call it the cluster entanglement mean field theory, and is described as follows.

For definiteness, consider a two-dimensional square lattice. See Fig. 1. A cluster in this case is a fundamental square of four spins. Let us focus on a particular cluster of four spins. These four spins interact among themselves by four interaction terms in H. They are the intra-cluster interactions. This basic unit, consisting of four spins, also interact with other spins in neighboring clusters via inter-cluster interaction terms in H. We first consider the intra-cluster terms. Just like in the case of the entanglement mean field theory, in every intra-cluster interaction term, we replace a unit random variable at a nearby dummy site by the square of an Ising random variable at that site. The difference is that the dummy site is now always chosen from the among the sites in the chosen cluster. This is just like in CMFT, where only the intra-cluster spins are involved in producing the terms of the form $m\sigma_{\vec{i}}$. So for the closen square cluster consisting of the sites formed by rows k, k-1 and columns l, l-1, for the intra-cluster term $\sigma_{k-1,l}\sigma_{k,l}$ in the Hamiltonian H, the site (k, l-1) can act as a dummy site, whereby we obtain the term $\sigma_{k-1,l}\sigma_{k,l}\sigma_{k,l-1}\sigma_{k,l-1}$. Similarly as in EMFT, the so-obtained term can be re-written as $A_{\chi}B_{\chi}$, with $A_{\chi} = \sigma_{k,l}\sigma_{k,l-1}$, and $B_{\chi} = \sigma_{k-1,l}\sigma_{k,l-1}$. We now replace B_{χ} by the unit multiple of the mean value C, and consequently, the contribution of this intracluster term to the cluster EMFT Hamiltonian \mathcal{H}_{CEMFT} is $-JC\sigma_{k,l}\sigma_{k,l-1}$. The entanglement coordination number of EMFT is absent in CEMFT, as the latter itself depends on the lattice geometry, and hence strenthens the approximation. The inter-cluster terms are taken care of by replacing them with effective fields at the corresponding spins of the chosen cluster, and these terms are exactly the same as in CMFT. The terms in H that are neither intra- not inter-cluster, do not appear in the considerations below, and are therefore ignored. Therefore, for a two-dimensional square lattice, with the chosen cluster, the cluster EMFT Hamiltonian is

$$\mathcal{H}_{CEMFT}^{sq} = -JC \sum_{\langle \vec{i}\vec{j} \rangle_{\chi}} \sigma_{\vec{i}} \sigma_{\vec{j}} - 2Jm \sum_{\vec{i}_{\chi}} \sigma_{\vec{i}} \qquad (5)$$

where the first sum runs over nearest neighbor sites of the chosen cluster, and the second runs over sites of the same. The factor 2 in the second term comes from the fact that we are considering a square lattice, so that every spin in the chosen cluster is connected (via an interaction term in H) to two spins in the neighboring clusters. Here, C denotes the nearest neighbor correlation of the lattice under consideration, and m the corresponding magnetization. One may similarly find the cluster EMFT Hamiltonian H_{CEMFT} for other models.

At this point, both C and m are undetermined. They are to be solved from the self-consistency relations (CEMFT equations) equating the correlation *and* the magnetization of the chosen cluster with the corresponding ones of the whole lattice:

$$C = \sum_{\mathcal{CF}(\mathcal{I})} \sigma_{\vec{i}} \sigma_{\vec{j}} \varrho_{CEMFT}^{\beta},$$

$$m = \sum_{\mathcal{CF}(\mathcal{I})} \sigma_{\vec{k}} \varrho_{CEMFT}^{\beta},$$
(6)

where \vec{i} and \vec{j} are any two nearest neighbor sites, and \vec{k} a particular site, in the chosen cluster. Here ρ_{CEMFT}^{β} is the cluster entanglement mean field canonical equilibrium state $\exp(-\beta H_{CEMFT})/Z_{CEMFT}$, $Z_{CEMFT} = \sum_{\mathcal{CF}(\mathcal{I})} \exp(-\beta H_{CEMFT})$) is the CEMF partition function. The CEMFT equations form a set of coupled self-consistency relations for C and m, and their nontrivial solution set exists only after a certain temperature, which is the critical temperature obtained from the cluster entanglement mean field theory.

The table below gives the predictions for the critical temperatures for the nearest neighbor Ising model in different lattice geometries and dimensions. In this paper, we have obtained the predictions from entanglement mean field theory and cluster entanglement mean field theory. The predictions from mean field theory can be obtained, e.g. from Refs. [3]. The predictions from cluster mean field theory are obtained in Refs. [6] and references therein. The exact and series results are obtained in Refs. [17] and references therein.

Lattice	MFT	EMFT	Improvement $(\%)$	CMFT	CEMFT	Improvement $(\%)$	Exact/Series
Linear	2	1	50	1.28	1.05	17.97	0
Hexagonal	3	2	67.57	2.335	1.21	63.53	1.52
Square	4	3	57.8	3.5	2.08	84.55	2.27
Triangular	6	5	42.37	5.64	3.99	82.5	3.64
Cubic	6	5	66.67	5.49	3.61	8.16	4.51

Table 1: A comparison of the critical temperatures obtained for the nearest neighbor Ising model in different lattices and geometries. Except for those in the two columns that mention the improvements, the numbers in the other columns are in units of $k_B T/J$. There are two columns with the heading "Improvement", of which the left one shows the improvement in the EMFT prediction over that from MFT, while the right one shows that for CEMFT over CMFT.

IV. CONCLUSION

We have proposed an entanglement mean field theory for dealing with classical interacting many-body models. Distinct from the mean field approach to interacting systems, the entanglement mean field one reduces the manybody parent Hamiltonian into a two-body one involving undetermined mean values of two-site physical parameters of the many-body parent. These undetermined parameters are determined via self-consistency equations between mean values of the two-body physical quantity of the reduced Hamiltonian and the many-body parent. We then generalize the concept to a cluster entanglement

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mean field theory where we work with a fundamental unit of the lattice. The self-consistency relations in this case are a set of coupled equations of single-site and two-site physical quantities. Solving these self-consistency equations lead to the predictions of critical temperatures of the models considered, which we then compare with the previous results. In all the cases considered, in the different geometries and dimensions, the predictions of the entanglement mean field theory are better than mean field theory (68% at most, and 42% at least), and the same of the cluster entanglement mean field theory are better than cluster mean field theory (85% at most, and 8% at least).

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