Order parameters in quasi-1D spin systems

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In this work we extend the notion of what is meant by a meanfield. For the purposes of this work meanfields are approximately maps - through some self consistency relation - of a complex, usually manybody, problem to a simpler more readily solvable problem. This mapping can then be solved to represent properties of the complex many body problem using some self consistency relations and the solution of the simpler problem. Prototypical examples of simpler meanfield problems (meanfield systems) are the single site and free particle problems - which are exactly solvable. Here we propose a new class of simple meanfield systems where the simple problem to be solved is a 1D spin chain. These meanfields are particularly useful for studying quasi-1D models, where there is a 3D system composed of weakly coupled 1D spin chains with the coupling in the transverse direction weaker then in the 1D direction. We illustrate this idea by considering meanfields for the Ising (of any coupling sign) and ferromagnetic Heisenberg models with one direction coupled much more strongly then the other directions (quasi-1D systems) which map at meanfield level onto the 1D Ising and 1D ferromagnetic Heisenberg models. We also consider more exotic models to illustrate other methods of solving 1D systems, namely the ferromagnetic N-state Potts model. Magnetic phase transition temperatures and are obtained for all three models, we see that they significantly differ from the usual meanfield estimates. Indeed if the 1D direction has coupling Γ and the transverse directions have coupling J with $\lambda \sim \frac{\Gamma}{J} \gg 1$ then regular meanfield would predict the transition temperature to be $k_B T_c \sim \Gamma$ for all three models while 1D meanfield predicts temperatures of $k_B T_c \sim \frac{\Gamma}{\log(\lambda)}$ for the Ising and Potts models and $k_B T_c \sim \frac{\Gamma}{\sqrt{\lambda}}$ for the ferromagnetic Heisenberg model. Cluster 1D (ladders etc.) meanfield extensions are also proposed.

I. INTRODUCTION

Meanfields have been very successfully and almost universally used as a first step towards the solution (understanding) of many complex manybody problems [1–5]. In a meanfield like solution of a complex problem we map a difficult manybody problem into a simpler one (a simpler system which can then be efficiently solved), solve the problem and solve for self consistency to relate the parameters of the solution of the simpler problem to the more complex many body problem to be solved or understood. The prototypical meanfield - simple - systems are the single site problem or the single particle problem. In the single particle case the complex system is mapped onto a quadratic Hamiltonian, through say a Hartree-Fock [5] meanfield, in a self consistent manner whereby properties of the complex model namely ground state energy, symmetry breaking, correlation functions may be often reliably computed to some accuracy from the Hartree-Fock problem [5]. In the single site problem - often a spin model is mapped onto a single spin problem which can be efficiently solved. Then self consistency is imposed through equating the parameters of the single site problem to the effects of the couplings to the neighboring spins and their magnetization [1]. In some cases, the single site problem may be extended, as in Dynamical Meanfield Theory (DMFT), to a single site and a bath whereby the frequency dependence (but not momentum dependence) of the Green's functions of the manybody system may be modeled self consistently through the dissipitative effects of the bath [6].

Here we propose another important simple system which may be effciently analyzed as a meanfield system - the 1D system. Indeed many 1D models are solvable through transfer matrix calculations [1, 7], Density Matrix Renormalization Group (DMRG) [8–10] methods , Jordan-Wigner fermionization [3, 5], or more generally the Bethe Ansatz (BA) methods [7, 11–13], and Exact Diagonalization (ED) techniques [14–16] to name a few. In this work we consider 3D spin systems where the coupling in one direction is much stronger then the coupling in the other two (quasi-1D systems). For these systems mapping the system to a 1D meanfield system and solving for self consistency is more efficient then regular meanfield (we verify this in part in Appendix A). We illustrate this idea through the 3D (quasi-1D) Ising model whose meanfield is the 1D Ising model (of either sign of coupling) in an external field (which is solvable by transfer matrix techniques) and the 3D (quasi-1D) ferromagnetic Heisenberg model whose meanfield is the 1D ferromagnetic Heisenberg model in an external field (which is solvable by BA techniques). We choose these two examples because of their simplicity clarity and because in both 3D and 1D these models are prototypical examples of models with magnetic phase transitions. We also illustrate the ideas through a more exotic related example the N-state ferromagnetic Potts model. We show significant differences between regular meanfield results and 1D meanfield results. Indeed assuming two couplings $\Gamma \gg J$ for longitudinal and transverse directions and $\lambda \sim \frac{\Gamma}{J} \gg 1$; then regular meanfield predicts a transition temperature of $k_B T_c \sim \Gamma$ for all three models while 1D improved meanfield shows that $k_B T_c \sim \frac{\Gamma}{\log(\lambda)}$ for the Ising and Potts models and $k_B T_c \sim \frac{\Gamma}{\sqrt{\lambda}}$ for the ferromagnetic Heisenberg model. Here k_B is the Boltzmann constant and T_c is the critical temperature for the magnetic phase transition. Cluster 1D meanfields are also proposed, which should systematically improve meanfield accuracy [1].

II. ISING MODEL

Consider a 3D quasi-1D ferromagnetic Ising model in an external field with the following Hamiltonian:

$$H_I = -\Gamma \sum_i \sigma^z(i)\,\sigma^z(i+\hat{z}) - J \sum_{\langle i,j\rangle, j\neq i\pm\hat{z}} \sigma^z(i)\,\sigma^z(j) + B\sum_i \sigma^z(i) \tag{1}$$

at a temperature β and $\langle i,j\rangle$ are nearest neighbors, here we will be interested in $\Gamma \gg J$ so that the 1D chains along the z-axis are more strongly coupled then the transverse plane. Antiferromagnetic Ising models are equivalent to ferromagnetic Ising models on bipartite lattices. so need not be considered Now consider the following meanfield Hamiltonian at unit temperature:

$$H_{MF} = \gamma \sum_i^N \sigma^z(i)\,\sigma^z(i+1) + h\sum_i \sigma^z(i) \tag{2}$$

Where for self consistency:

$$\gamma = \beta\Gamma,\ h = \beta J\mathcal{N}m - \beta B \tag{3}$$

here $\mathcal{N} \sim 2(d-1)$ is the number of nearest neighbors in the weakly coupled directions and $d = 3$ is the dimension of the system. Then we know that the magnetization m in the thermodynamic limit for the Hamiltonian in Eq. (2) at unit temperature is given by 1 [1]:

$$m = \frac{\sinh(h)}{\left[\exp(-4\gamma) + (\sinh(h))^2\right]^{1/2}} \tag{4}$$

This is an exact result (using the transfer matrix formalism) [1, 7]. Now we substitute the meanfield relations in Eq. (3) and obtain:

$$m = \frac{\sinh(\beta J\mathcal{N}m - \beta B)}{\left[\exp(-4\beta\Gamma) + (\sinh(\beta J\mathcal{N}m - \beta B))^2\right]^{1/2}} \tag{5}$$

Setting $B = 0$ and linearizing to find the phase transition temperature we have that:

$$\begin{aligned} m &= \exp(2\beta\Gamma)\,\beta J\mathcal{N}m, \\ 1 &= \exp(2\beta\Gamma)\,\beta J\mathcal{N} \end{aligned} \tag{6}$$

leads to magnetism. Taking the logarithm of both sides we see that:

$$2\beta\Gamma = -\log(\beta J\mathcal{N}) \tag{7}$$

Introducing

$$\lambda = \frac{\Gamma}{J\mathcal{N}} \gg 1 \tag{8}$$

We get that:

$$2\lambda = -\frac{\log(\beta J\mathcal{N})}{\beta J\mathcal{N}} \tag{9}$$

We now write:

$$\beta_0 J\mathcal{N} = \frac{1}{2\lambda} \tag{10}$$

Then:

$$-\frac{\log(\beta J\mathcal{N})}{\beta J\mathcal{N}} \cong \frac{\log(2\lambda)}{\beta J\mathcal{N}} \tag{11}$$

This means that:

$$\beta_1 J\mathcal{N} = \frac{1}{2\lambda\log(2\lambda)} \tag{12}$$

In general we can iterate the solution through the relation (though Eq. (12) is often enough):

$$\beta_{n+1} J\mathcal{N} = -\frac{1}{2\lambda\log(\beta_n J\mathcal{N})} \tag{13}$$

We note that the usual meanfield equations the phase transition temperature can be found through the following relationship:

$$2\beta\Gamma + \beta J\mathcal{N} = 1 \tag{14}$$

Which are much worse as it predicts:

$$\beta J\mathcal{N} = \frac{1}{2\lambda + 1} \tag{15}$$

which is significantly different, for large λ, then Eq. (12), see Appendix A.

III. N STATE POTTS MODEL

We focus on the ferromagnetic Potts model. We write:

$$H_{Pott} = -\Gamma\sum_i \delta(n(i), n(i+\hat{z})) - J\sum_{\langle i,j\rangle, j\neq i\pm\hat{z}} \delta(n(i), n(j)) + B\sum_i \delta(n(i), 1) \tag{16}$$

Where $n(i)$ is the state of the i'th unit, with $n(i) = 1, 2..., N$. We now write the Hamiltonian of the meanfield system:

$$H_{Pott} = -\Gamma\sum_i \delta(n(i), n(i+1)) - \mathcal{B}\sum_i \delta(n(i), 1) \tag{17}$$

Then we write the transfer matrix [1, 7] of the system as:

$$\begin{aligned} T = & \left|V\right\rangle\left\langle V\right| + \left(\exp\left(\mathcal{B}\right) - 1\right)\left[\left|V\right\rangle\left\langle 1\right| + \left|1\right\rangle\left\langle V\right|\right] \\ & + \left(\exp\left(\Gamma\right) - 1\right)\sum_{i=2}^{N}\left|i\right\rangle\left\langle i\right| + \\ & + \left(\exp\left(\Gamma + 2\mathcal{B}\right) - 2\exp\left(\mathcal{B}\right) + 1\right)\left|1\right\rangle\left\langle 1\right| \end{aligned} \tag{18}$$

Where we introduce the un-normalized vector

$$\left|V\right\rangle = \sum_{i=1}^{N}\left|i\right\rangle \tag{19}$$

Now we look for the biggest eigenvalue of the transfer matrix [1, 7] using the ansatz:

$$\begin{aligned} & E\left(a\left|1\right\rangle + b\left|V\right\rangle\right) \\ & = T\left(a\left|1\right\rangle + b\left|V\right\rangle\right) \end{aligned} \tag{20}$$

Now we linearIze everything for small $\mathfrak{B}$ in order to find the magnetic phase transition and write:

$$\begin{pmatrix} \left(\exp\left(\beta\Gamma\right) - \left(2\exp\left(\beta\Gamma\right) - 1\right)\beta\mathcal{B}\right) & \left(\left(N-2\right) + 2\exp\left(\beta\Gamma\right)\right)\beta\mathcal{B} \\ \beta\mathcal{B} & \left(N - 1 + \exp\left(\beta\Gamma\right) + \beta\mathcal{B}\right) \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = E\begin{pmatrix} a \\ b \end{pmatrix} \tag{21}$$

For a full calculation to all orders see Appendix B. Now we treat the matrix proportional to $\beta\mathcal{B}$ as a perturbation and we write:

$$\begin{pmatrix} \exp\left(\beta\Gamma\right) & 0 \\ 0 & \left(N - 1 + \exp\left(\beta\Gamma\right)\right) \end{pmatrix} + \beta\mathcal{B}\begin{pmatrix} \left(2\exp\left(\beta\Gamma\right) - 1\right) & \left(\left(N-2\right) + 2\exp\left(\beta\Gamma\right)\right) \\ 1 & 1 \end{pmatrix} \tag{22}$$

Then

$$E \cong \left(N - 1 + \exp\left(\beta\Gamma\right)\right) + \beta\mathcal{B} \tag{23}$$

$$b \cong 1 \tag{24}$$

$$a \cong \frac{\beta\mathcal{B}\left(N + 2\exp\left(\beta\Gamma\right) - 2\right)}{N - 1} \tag{25}$$

and

$$M \cong \frac{2a}{N} = \frac{2\beta\mathcal{B}\left(N + 2\exp\left(\beta\Gamma\right) - 2\right)}{\sqrt{N}\left(N-1\right)} \tag{26}$$

is the magnetization. This then means that at meanfield:

$$\begin{aligned} & \mathcal{B} = M\mathcal{N}J \\ & \Rightarrow 1 = \frac{2\beta\mathcal{N}J\left(\left(N-2\right) + 2\exp\left(\beta\Gamma\right)\right)}{N\left(N-1\right)} \end{aligned} \tag{27}$$

Now we will assume that $\beta\mathcal{N}J \ll 1$ so that $(N-2) \ll 2\exp\left(\beta\Gamma\right)$ as such we obtain:

$$\begin{aligned} 1 &= \frac{4\beta\mathcal{N}J\exp\left(\beta\Gamma\right)}{N\left(N-1\right)} \\ \beta\Gamma &= \log\left(\frac{N\left(N-1\right)}{4\beta\mathcal{N}J}\right) \\ \lambda &= \frac{\log\left(\frac{N(N-1)}{4\beta\mathcal{N}J}\right)}{\beta J\mathcal{N}} \cong \frac{\log\left(N\left(N-1\right)/4\right)}{\beta J\mathcal{N}} \\ \beta J\mathcal{N} &\cong \frac{\log\left(N\left(N-1\right)/4\right)}{\lambda} \end{aligned} \tag{28}$$

Iterating we get that:

$$\begin{aligned} 1 &= 2\frac{\log\left(N\left(N-1\right)/4\right)}{\lambda}\frac{\left(\left(N-2\right) + 2\exp\left(\beta\Gamma\right)\right)}{N\left(N-1\right)} \\ \beta\Gamma &\cong \frac{1}{2}\log\left(\frac{\lambda N\left(N-1\right)}{2\log\left(N\left(N-1\right)/4\right)} - N + 2\right) \end{aligned} \tag{29}$$

IV. FERROMAGNETIC HEISENBERG MODEL

We consider the anisotropic 3D (quasi-1D) ferromagnetic Heisenberg model with the following Hamiltonian:

$$\begin{aligned} H = & -\Gamma\sum_{i}\vec{\sigma}\left(i\right)\cdot\vec{\sigma}\left(i+\hat{z}\right) \\ & - J\sum_{\langle i,j\rangle, j\neq i\pm\hat{z}}\vec{\sigma}\left(i\right)\cdot\vec{\sigma}\left(j\right) + B\sum_{i}\sigma_i^z \end{aligned} \tag{30}$$

with $\mathcal{J} \gg J$. Now we consider the following meanfield Hamiltonian (which happens to be the Heisenberg model in an external field and as such solvable by BA techniques [11, 12]):

$$H_{MF} = -\Gamma\sum_{i}\vec{\sigma}\left(i\right)\cdot\vec{\sigma}\left(i+1\right) - h\sum_{i}\sigma^z\left(i\right) \tag{31}$$

with

$$h = \mathcal{N}J\mathcal{M} - B \tag{32}$$

Where $\mathcal{M}$ will be chosen self consistently that is:

$$\mathcal{M} = \left\langle\sigma^z\left(i\right)\right\rangle_{H_{MF}} \tag{33}$$

We will now solve Eqs. (31) and (33) and find the critical transition temperature where $\mathcal{M}$ vanishes. This will be an extended meanfield treatment of the Hamiltonian in Eq. (30). Indeed the magnetic susceptibility χ can be used to determine phase boundaries. We have that for the ferromagnetic Heisenberg model at temperature T the susceptibility is given by [11, 12]:

$$\chi = \mathcal{J}^{-1}\left(\frac{1}{6}\left(\frac{\Gamma}{T}\right)^2 + 0.581\left(\frac{\Gamma}{T}\right)^{3/2} + 0.68\left(\frac{\Gamma}{T}\right)\right) + ... \tag{34}$$

Now to determine the phase transition temperature between magnetic and non-magnetic phase we use the relationship:

$$\begin{aligned} \chi h &= \mathcal{M} \\ \chi \mathcal{N} J \mathcal{M} &= \mathcal{M} \\ \chi \mathcal{N} J &= 1. \end{aligned} \tag{35}$$

Where we have set $B = 0$ to find the phase transition. As such for the phase transition between magnetic and non-magnetic we write:

$$\frac{\mathcal{N}J}{\Gamma}\left(\frac{1}{6}\left(\frac{\Gamma}{T}\right)^2 + 0.581\left(\frac{\Gamma}{T}\right)^{3/2} + 0.68\left(\frac{\Gamma}{T}\right)\right) = 1 \tag{36}$$

Now we have that

$$\begin{aligned} &\frac{\mathcal{N}J}{\Gamma}\left(\frac{1}{6}\left(\frac{\Gamma}{T}\right)^2 + 0.581\left(\frac{\Gamma}{T}\right)^{3/2} + 0.68\left(\frac{\Gamma}{T}\right)\right) \\ &\cong \frac{1}{6\lambda}\left(\frac{\Gamma}{T}\right)^2 \end{aligned} \tag{37}$$

This means that at first approximation for the critical temperature:

$$T_0 \cong \Gamma\left(\frac{1}{6\lambda}\right)^{1/2} \tag{38}$$

Now we write:

$$\begin{aligned} &\frac{\mathcal{N}J}{\Gamma}\left(\frac{1}{6}\left(\frac{\Gamma}{T}\right)^2 + 0.581\left(\frac{\Gamma}{T}\right)^{3/2} + 0.68\left(\frac{\Gamma}{T}\right)\right) \\ &\cong \frac{\mathcal{N}J}{\Gamma}\left(\frac{1}{6}\left(\frac{\Gamma}{T_0}\right)^2 + 0.581\left(\frac{\Gamma}{T_0}\right)^{3/2} + 0.68\left(\frac{\Gamma}{T_0}\right)\right) \end{aligned} \tag{39}$$

As such the second approximation for the critical temperature gives:

$$T_1 \cong \Gamma\sqrt{\frac{1}{6\lambda}\left[1 - 2.23\left(\frac{1}{\lambda}\right)^{1/4} - 1.67\left(\frac{1}{\lambda}\right)^{1/2}\right]} \tag{40}$$

We can continue to iteratively solve the problem for the critical temperature more and more accurately using the formula (though Eq. (40) is often sufficient):

$$T_{n+1} \cong \Gamma\sqrt{\frac{1}{6\lambda}\left[1 - \frac{1}{\lambda}\left[0.581\left(\frac{\Gamma}{T_n}\right)^{3/2} - 0.68\left(\frac{\Gamma}{T_n}\right)\right]\right]} \tag{41}$$

V. CONCLUSIONS

In this work we have extended the notion of the meanfield. We have proposed a new class of meanfield models where 1D systems are the meanfield problems to be solved. This combined with self consistency relations may be used to efficiently solve for properties of anisotropic 3D or quasi-1D systems - where one direction is much more strongly coupled then the other. In this work we have illustrated this idea with the Ising and ferromagnetic Heisenberg models which are solvable by transfer matrix and Bethe Ansatz techniques respectively and found transition temperatures as preliminary results. We also studied a more exotic model - the Potts model. We found significantly different results then regular meanfield. Indeed we found magnetic phase transition temperatures of $k_B T_c \sim \frac{\Gamma}{\log(\lambda)}$ for the Ising and Potts models and $k_B T_c \sim \frac{\Gamma}{\sqrt{\lambda}}$ for the ferromagnetic Heisenberg model, where as regular meanfield predicts $k_B T_c \sim \Gamma$ for all three models. In future works it would be of interest to extend these results to many other quasi-1D systems systematically. Furthermore it would be of interest to study cluster 1D meanfields, where a cluster of 1D systems is chosen as the meanfield system to be solved. The accuracy of the calculation is systematically improved with cluster size in cluster 1D meanfields.

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Appendix A: Onsager solution

We note that the Onsager relation for $d = 2$ ($\mathcal{N} = 2$) is that the critical temperature is given by [1, 17]:

$$\begin{aligned} \sinh(2\beta J)\sinh(2\beta\Gamma) &= 1 \\ \exp(2\beta\Gamma)\cdot\beta J &\cong 1 \end{aligned} \tag{A1}$$

This is the exact same relationship as in Eq. (6) for $\mathcal{N} = 1$, which means that:

$$\beta J = \frac{1}{2\lambda\log(2\lambda)} + ... \tag{A2}$$

This means the meanfield is accurate within a factor of two while the regular meanfield is off by $\sim \log(2\lambda)$ for large λ showing significant improvement of our approach over regular meanfield in the limit of strong anisotropy or nearly 1D systems.

Appendix B: N-state Potts model in an external Field at unit temperature

Now we look for the biggest eigenvalue using the ansatz in Eq. (20). This means that:

$$\begin{pmatrix} (\exp(J+2B)-\exp(B)+1) & ((N-2)[\exp(B)-1]+\exp(J+2B)-\exp(J)) \\ [\exp(B)-1] & (N-2+\exp(B)+\exp(J)) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = E \begin{pmatrix} a \\ b \end{pmatrix} \tag{B1}$$

This means that

$$\det \begin{bmatrix} (\exp(J+2B)-\exp(B)+1-E) & ((N-2)[\exp(B)-1]+\exp(J+2B)-\exp(J)) \\ [\exp(B)-1] & (N-2+\exp(B)+\exp(J)-E) \end{bmatrix} = 0 \tag{B2}$$

As such:

$$E^2 - E[\exp(J+2B)+N-1+\exp(J)] + \exp(2J+2B) + [N-1][\exp(J+2B)-\exp(2B)+\exp(B)] = 0 \tag{B3}$$

As such (since we want the biggest eigenvalue):

$$E_+ = \frac{[\exp(J+2B)+N+\exp(J)-1]+\sqrt{\Delta(J,B,N)}}{2} \tag{B4}$$

Where

$$\Delta(J,B,N) = [\exp(J+2B)-N+1+\exp(J)]^2 - 4[\exp(2J+2B)+[N-1][\exp(B)-\exp(2B)-\exp(J)]] \tag{B5}$$

Now we have that

$$\begin{aligned} \frac{a}{b} &= \frac{E_+ - N + 2 - \exp(B) - \exp(J)}{\exp(B)-1} \\ &= \frac{\exp(J+2B)+\sqrt{\Delta(J,B,N)}}{2(\exp(B)-1)} - \frac{1}{2} \end{aligned} \tag{B6}$$

Now we have that the normalization of the vector is

$$\| a\,|1\rangle + b\,|V\rangle \| = Nb^2 + a^2 + 2ab \tag{B7}$$

Therefore the magnetization is given by:

$$M = \frac{a^2+2ab}{Nb^2+a^2+2ab} \tag{B8}$$

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