Modern Physics Letters B20:649-654, (Vol. 20, No. 11, 10th May 2006)

Long Range 1-d Potential at border of Thermodynamic Limit

O. Shanker
http://www.geocities.com/oshanker *

Received 26 July 2005

In this work we consider new forms of the 1-d long range potential close to the thermodynamic limit. We also look at the potential close to the transition from long range order to short range order. We find an interesting duality between the two potentials, based on Dyson's sufficiency conditions for the existence of a phase transition. An important conclusion of our study is that the very long range nature of the potential causes Monte Carlo simulations to reach an apparent, but misleading, convergence. Thus, one needs to exercise great caution in deriving conclusions from such studies.

Keywords: Thermodynamic Limit, 1-d Phase Transitions, Long Range Potential

1. Introduction

Phase transitions in one dimensional spin models show a rich diversity of behaviour [1,2,3,4,5]. The study of the power law potential [6,7,8], where the interaction varies with the distance r as $1/r^{\alpha}$, has been particularly detailed. It would be interesting to consider extensions to other potential forms. It has been shown for power law potentials that phase transitions exist when $0 \leq \alpha \leq 2$. However, when $0 \leq \alpha \leq 1$, system properties like the free energy do not behave extensively, i.e., they increase faster than N as $N \rightarrow \infty$, where N is the number of spins in the system. This region is the mean field region. $1 < \alpha \leq 2$ is the region with long range order, and $\alpha = 2$ marks the transition from long range order to short range order. In this paper I investigate some potentials which are not of the power law form, and which probe regions close to interesting values of α. I first derive a potential (denoted potential A) which is extensive, and which nevertheless decreases more slowly as r increases than any power law potential which is also extensive (this is the $\alpha \searrow 1$ region). I then derive a potential (denoted potential B) which has long range order, and which nevertheless decreases more slowly as r increases than any power law potential except $\alpha = 2$ (this is the $\alpha \nearrow 2$ region). We shall see that these potentials are related in an intriguing manner. I then study the potentials in the context of a Ising model spin chain, using a simple extension of mean field theory. I perform some Monte Carlo numerical studies. The Monte Carlo simulations seem to converge

*oshanker@gmail.com

quickly. However, I show that the seeming convergence is misleading, and in fact the Monte Carlo simulations are converging for the wrong model. This is related to the very long range nature of the potentials we are considering. I also show that one of the potentials is apparently intractable using present Monte Carlo techniques, even the rather sophisticated techniques [9,10,11]. Finally, I present the conclusions.

2. Derivation of the potential

For definiteness, we will consider the one-dimensional Ising model with the Hamiltonian (with N spins and periodic boundary conditions)

$$H = -\frac{1}{2}\sum_{i,j} J(r(i,j))s_i s_j \tag{1}$$

where s_i are the spin variables, $r(i,j) = |i-j|$, and $J(r(i,j))$ are the couplings between the spins. We will specialise to ferromagnetic couplings, i.e., all the J are positive. When the $J(r(i,j))$ have the behaviour $1/r^{\alpha}$, we have the power law potential. We wish to find a potential which preserves extensivity, while decreasing more slowly with increasing r than any extensive power law potential. At zero temperature, the energy per spin is proportional to

$$\rho = \sum_{i,j} J(r(i,j)), \tag{2}$$

and hence extensivity requires that ρ be finite. This requirement is the one which makes $\alpha = 1$ the transition point for the power law potential. To meet the requirements, we have to introduce logarithmic terms in the r dependence of J. As will become clear from the discussion which follows, it will be convenient to use the base 2 for the logarithms. We would be tempted to make the ansatz

$$J(r) = J(1)/(r * log(r) * log(log(r)) * .. * log^{(k)}(r)), \tag{3}$$

where we use the notation $log^{(k)}(r)$ for the k-fold iteration of taking the log. However, no matter how large we make k, ρ always diverges for the above form of the potential! The result follows from the observation that the terms constitute a convex function of r, and hence one can find a lower bound for ρ in terms of the integral

$$\int (dr/(r * log(r) * log(log(r)) * .. * log^{(k)}(r))). \tag{4}$$

The integral can be evaluated by observing that

$$d(log^{(k+1)}(r))/dr = (log(e))^{m+1}/(r * log(r) * log(log(r)) * .. * log^{(k)}(r))) \tag{5}$$

and hence ρ diverges as $log^{(k+1)}(N)$. It may be mentioned that if we raise the $log^{(k)}(r)$ term to the power α, then the series converges for $\alpha > 1$ and diverges for $\alpha \leq 1$. Hence we may choose $\alpha > 1$ and use the potential with the log terms. However, it would be aesthetically more satisfying if we could avoid the introduction of α (after all, the power law has exactly the same behaviour, and in fact is a special case of the general relation presented above for the convergence of ρ). In fact, we can find a potential which decreases more slowly than any of the above potentials as r increases. The potential is of the form in Eq. (3), where, instead of taking k fixed, we do the iteration of the log as long as the result is greater than one. We call this potential A. We have to show, firstly, that the sum then converges, and, secondly, that the system with the potential described indeed has a phase transition. The convergence of the sum follows from the fact that an upper limit can be set on ρ in terms of a sum of integrals of the form Eq. (4). In what follows, we use units such that $J(1) = 1$. Let us first divide the sum into partial sums, in terms of the integers $h(j)$, where $h(0) = 1$, and $h(n+1) = 2^{h(n)}$. Then the partial sum from $h(j)$ to $h(j+1)$ is bounded from above by $1/log(e)^j$, and hence the total sum is bounded by $log(e)/(log(e) - 1)$. It is worth noting that the convergence is very slow, since the $h(j)$ increase very fast with j. The value of ρ is equal to 2.86. Table 1 illustrates the extreme slowness for the convergence of ρ.

Table 1. Slow convergence of the sum ρ for potential A. The sum is expressed in units where $J(1) = 1$.

Serial Number j	Number of terms $h(j)$	Value of sum ρ
1	1	1.00
2	2	1.50
3	4	1.84
4	16	2.12
5	65536	2.34
	∞	2.86[a]

[a] Estimated using integral Eq. (4).

Having shown that the system with potential A is extensive in the thermodynamic limit, we now have to show that it has a phase transition. This is easily done by using the result of Ref. 2. It is shown there that a phase transition exists if the potential is positive and monotonically decreasing with increasing r, and satisfies two sum rules. The first rule is that ρ defined above should converge. We have already proved that. The second condition is that the sum

$$\varrho = \sum_{i,j} log(log(r(i,j))/(r(i,j)^3 J(r(i,j))) \tag{6}$$

should also converge. For potential A, using the techniques discussed above one can easily show that ϱ converges to the value 5.63. Thus, we have achieved the set goal. It is satisfying that the potential we derived does not depend on arbitrary parameters like α.

Let us now derive Potential B, which is close to the transition from long range to short range order. To guide us in the choice of form for the potential, we note that for the power law, the transition limit occurs because the condition Eqn. 6 diverges. We thus have to find a potential which is close to the power law $1/r^2$, but which has ϱ finite. Using arguments similar to the one we used for deriving potential A from the sum condition for ρ, we find that the finiteness of ϱ can be satisfied if we choose

$$J(r) = \sum_{i,j} log(log(r)) * log(r) * log(log(r)) * .. * log^{(k)}(r)/r^2 \tag{7}$$

where the logs are iterated as long as they remain greater than one. The proof that potential B satisfies the Dyson sum conditions is trivial: the ϱ sum for potential B is equal to the ρ sum for potential A, and the ρ sum for potential B is equal to the ϱ sum for potential A! Once again, it is satisfying that the potential does not depend on parameters, and furthermore, the duality of the potentials under the Dyson sum rules is intriguing!

3. Extended Mean Field Theory

We have studied the potentials using a simple extension of mean field theory, where the nearest neighbour spin correlations are treated exactly, and the other spin correlations are treated under the mean field approximation. For potential A, which is close to the mean field region $0 \leq \alpha \leq 1$, this should be a good approximation. To present the results, let us denote (for both potentials)

$$J' = 2 \sum_{j-i>1} J(r). \tag{8}$$

In other words, $J' = 2(\rho - J(1))$. If we denote the magnetisation per spin by m, then the self-consistency condition for m is

$$m = \frac{sinh(\beta J' m)}{\sqrt{sinh^2(\beta J' m) + e^{-4\beta J(1)}}} \tag{9}$$

where β is the inverse temperature. This has non-zero solutions for m only when

$$\beta J' > e^{-2\beta J(1)} \tag{10}$$

For potential A this predicts the critical temperature T_c to be 5.2 in units where $J(1) = 1$. For potential B the critical temperature is predicted to be 10.5.

4. Monte Carlo study and pseudo-convergence

Fig. 1 shows Monte Carlo results for potential A, for system sizes $N = 5000$ and $N = 10000$. We plot the square of the magnetization density as a function of the inverse temperature. The convergence seems to be good. However, Table 1 shows that for any reasonable system sizes, there is a large error in the calculation of the potential itself. This is likely to result in large errors for the Monte Carlo estimates of various quantities. Because we can use only a finite number of terms while the potential gets significant contiributions from spins very far away, the T_c that one gets from the Monte Carlo estimate is likely to be too small. Indeed, we find the

Monte Carlo estimate to be about 3.33, as compared to the prediction above of 5.2. It seems difficult to significantly reduce the Monte Carlo error, given the slow rate of convergence of the spin sum for potential A. For potential B we carried out similar studies, and found that there appears to be a peak in the magnetic susceptibility at a temperature of 10.5. This system is more tractable than the first one.

5. Conclusions

In conclusion, we have derived two potentials which probe the regions close to the thermodynamic limit and the region close to the transition from long range order to short range order. We presented the properties of the potentials, and pointed out the extremely slow rate of convergence for the sums appearing in the calculations. This makes the numerical estimates using Monte Carlo methods difficult, if not intractable for Potential A. It also brings out the need to exercise caution in interpreting the Monte Carlo results, since they seem to show good convergence, which is really not physical and is an indication of the very long range We presented some analytical estimates for the magnetisation and critical temperature. We saw an interesting duality relationship between the potentials in the two regimes. The duality arises from the Dyson sufficiency conditions for the existence of a phase transition.

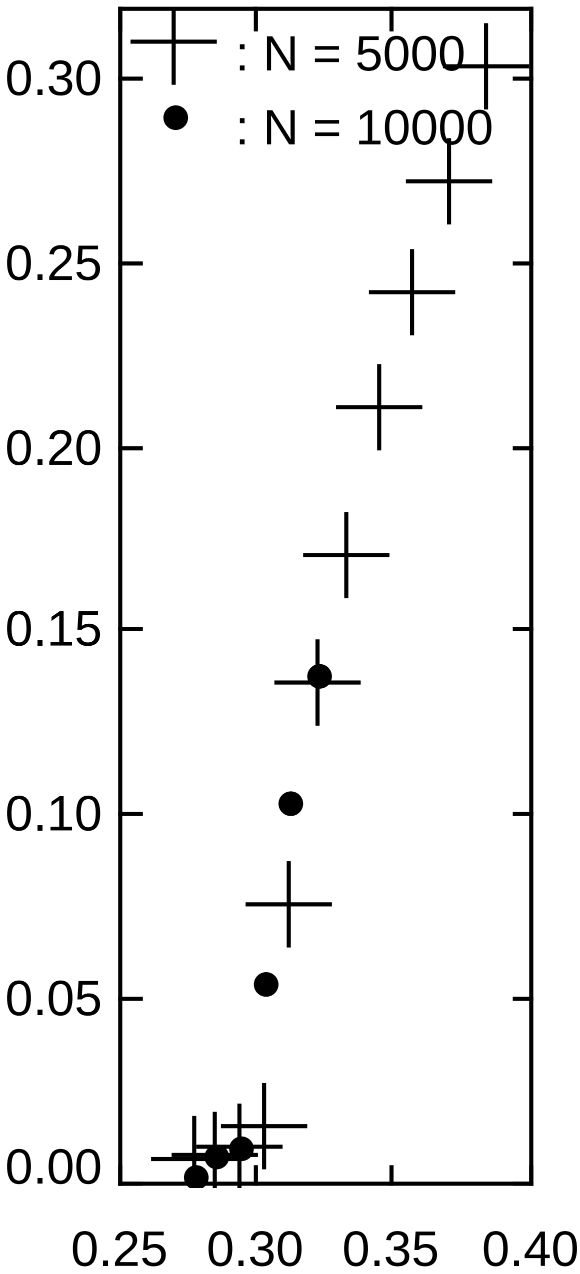

Fig. 1. Scaled order parameter vs inverse temperature for potential A.

1. D. Ruelle, *Commun. Math. Phys.* **9**, 267 (1968).
2. F. J. Dyson, *Commun. Math. Phys.* **12**, 91 (1969).
3. J. Frohlich and T. Spencer, *Commun. Math. Phys.* **84**, 87 (1982).

4. M. Aizenman, J. T. Chayes, L. Chayes and C. M. Newman, *J. Stat. Phys.* **50**, 1 (1988).
5. J. Z. Imbrie and C. M. Newman, *Commun. Math. Phys.* **118**, 303 (1988).
6. E. Luijten and H. Messingfeld, *Phys. Rev. Lett.* **86**, 5305 (2001).
7. S. A. Cannas, A. C. N. de Magalhaes and F. A. Tamarit, *Phys. Rev.* **B61**, 1152 (2000).
8. K. Uzelac and Z. Glumac, *Phys. Rev. Lett.* **85**, 5255 (2000).
9. E. Luijten and H. W. J. Blote, *Int. J. Mod. Phys.* **C6**, 359 (1995).
10. R. H. Swendson and J.-S. Wang, *Phys. Rev. Lett.* **58**, 86 (1987).
11. U. Wolff, *Phys. Rev. Lett.* **62**, 361 (1989).