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Development of a Phase Transition for a Rigorously Solvable Many-Body System*

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The ferromagnetic transition is considered in detail for the Heisenberg Hamiltonian with all spins coupled equally. For this special model the statistical problem is solved exactly. The transition develops very slowly as the number N of particles in the system is increased; the spin order at the nominal Curie temperature is proportional to $N^{-1/4}$. The order in the most probable state differs from the mean value of the order, except for $N \rightarrow \infty$. The connections are studied with the molecular-field, spin-wave, and self-consistent approximations. The failure of the self-consistent approximation is relatively severe as compared with the nearest-neighbor problem. The antiferromagnetic ground state is very close in energy to the Néel state.

INTRODUCTION

So few phase-transition problems are solvable that a certain interest may perhaps attach to any model, however artificial, which is solvable exactly. In this paper we study the development of the ferromagnetic transition for a special model. There are features to the results which were not entirely anticipated by us.

The eigenvalues of the Heisenberg spin Hamiltonian are known exactly for the special case of a uniform interaction which couples all spins $\mathbf{S}_i$ to all other spins $\mathbf{S}_j$ by an exchange interaction J:

$$H' = -2J \sum_{i>j} \mathbf{S}_i \cdot \mathbf{S}_j = -J(\mathcal{S}\cdot\mathcal{S} - \sum_i S_i^2), \tag{1}$$

where $\mathcal{S} \equiv \sum_i \mathbf{S}_i$ is the total-spin operator. It is convenient to write, for a system of N spins S,

$$H = -J\mathcal{S}\cdot\mathcal{S} + JNS(NS+1), \tag{2}$$

for now the ground-state energy is zero.

For $S=\frac{1}{2}$ the eigenvalues of H are

$$\lambda_p = J\{(N+1)p - p^2\}, \tag{3}$$

where the pth eigenvalue belongs to total spin $\mathcal{S}=\frac{1}{2}N-p$. The result is independent of the geometry of the spins. We may define a wave vector k if, for example, we arrange the spins on a ring. The excitation energy for $p=1$ is $\lambda_1-\lambda_0=NJ$, so that the dispersion relation for one-magnon excitation is $\omega_k=NJ$, a constant, except for the state $k=0$ which belongs to $p=0$, so that $\omega_0=0$. The effect of magnon-magnon interactions is in the term in p^2 in λ_p. We see that the energy of the pth excitation is $\lambda_p-\lambda_{p-1}=J(N-2p+2)$; the higher the order of the excitation, the lower is the incremental excitation energy.

The degeneracy of the pth level is easily found[1]:

$$G_p = (N-2p+1)^2 \frac{N!}{(N-p+1)!p!}, \tag{4}$$

a standard result. The partition function is

$$Z = \sum_{p=0}^{\frac{1}{2}N} G_p e^{-\beta\lambda_p}, \tag{5}$$

with $\beta \equiv 1/k_BT$. We assume that N is an even number.

INFINITE SYSTEMS

If we neglect terms of order $1/N$ and $1/p$, and write the Stirling approximation as $x! \cong x^x e^{-x}$, we have

$$Z \cong \sum_{p=0}^{\frac{1}{2}N} \exp\{N\ln N - (N-p)\ln(N-p) - p\ln p - \beta J(Np-p^2)\}. \tag{6}$$

The exponent is a maximum when $\partial\{\cdots\}/\partial p=0$, so that the most probable value of p is given by

$$\mathrm{lng}(N-p) - \ln p - N\beta J + 2p\beta J = 0. \tag{7}$$

We introduce as a measure of the order of the system the quantity η defined by

$$\eta \equiv (N-2p)/N; \quad \alpha \equiv N\beta J \equiv NJ/k_BT. \tag{8}$$

To get a feeling for η, note that $N-p$ is the number of *un*reversed spins and p is the number of reversed spins. Their difference is $N-2p$. The maximum possible value of η is 1; the minimum possible value is zero, because the minimum value of $\mathcal{S}$ is zero. Now (7) may be rewritten as

$$\ln[(1+\eta)/(1-\eta)] = \alpha\eta \tag{9}$$

or

$$\tanh\tfrac{1}{2}\alpha\eta = \eta. \tag{10}$$

This transcendental equation has a nonzero root only for $\alpha > \alpha_c$, where $\alpha_c=2$. From the definition of α in (8) we have

$$k_BT_c = \tfrac{1}{2}NJ. \tag{11}$$

This defines the Curie temperature. For T slightly below T_c, we establish by series expansion of (9) or (10) that

$$\tfrac{1}{3}\eta^2 \cong (T_c-T)/T_c. \tag{12}$$

For $T=0$, we find from (10) that $\eta=1$: The order is

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[1] J. H. Van Vleck, *Electric and Magnetic Susceptibilities* (Clarendon Press, Oxford, 1932), pp. 323–324.

complete. For $T>T_c$, we find $\eta=0$ or $p=\frac{1}{2}N$: This is called complete disorder.

The internal energy is constant for $T>T_c$ and is equal to $\frac{1}{4}N^2J$. This is also its value just below T_c. The heat capacity (as T increases through T_c) drops suddenly at T_c from $\frac{3}{2}Nk_B$ to 0, and remains zero above T_c. The magnetic moment may be defined as $g\mu_B\langle\mathcal{S}_z\rangle$. If we add to the Hamiltonian a term $-g\mu_B\mathcal{S}_z\mathcal{H}$, where $\mathcal{H}$ is the magnetic field intensity, we find that the most probable value of η for $T>T_c$ is now given by (for $\eta\ll 1$):

$$\eta=(g\mu_B/2k_B)[\mathcal{H}/(T-T_c)], \tag{13}$$

so that the magnetic susceptibility is

$$\chi=\frac{N}{V}\frac{\mu^2}{k_B}\frac{1}{T-T_c}, \tag{14}$$

where V is the volume. This is of the form of the Curie-Weiss law.

The results (10), (11), (12), (14) for the infinite system are identical with those of the standard molecular-field approximation. In one statement of the molecular-field approximation the interaction is taken in the Ising form, but with an infinite-range interaction. Thus the Hamiltonian is

$$H_I'=-2J\sum_{i>j}S_i^zS_j^z=-J\mathcal{S}_z^2+J\sum_i(S_i^z)^2. \tag{15}$$

The eigenvalues for $S=\frac{1}{2}$ are, referred to $\lambda_0=0$,

$$\lambda_r=rJ(N-r), \tag{16}$$

where the rth eigenvalue belongs to $\mathcal{S}_z=\frac{1}{2}N-r$. The degeneracy of this level is

$$G_r=N!/(N-r)!r!, \tag{17}$$

somewhat different from (4). The partition function on the Ising model is

$$Z_I=\sum_{r=0}^{N}G_re^{-\beta\lambda_r}. \tag{18}$$

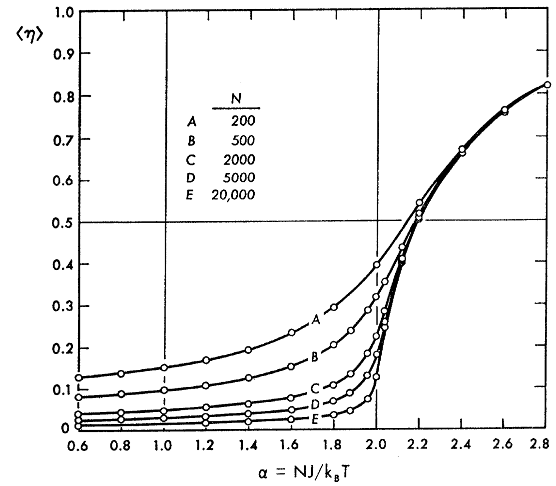

FIG. 1. Order parameter η as a function of the normalized reciprocal temperature for various numbers of particles.

To the previous order in the Stirling approximation we have

$$Z_I\cong\sum_{r=0}^{N}\exp\{N\ln N-(N-r)\ln(N-r)-r\ln r-\beta J(Nr-r^2)\}, \tag{19}$$

identical with (6) except for the different upper limit. The most probable value of r in this approximation is identical with the most probable value of p found in (7), and to the same approximation all the other results are identical for the two models. Differences appear in higher orders, as discussed in Appendix A.

EXACT NUMERICAL SOLUTIONS FOR FINITE NUMBERS OF SPINS

The relative simplicity of the partition function (5) with the exact expressions (3) and (4) for the energy eigenvalues and the degeneracy induced us to program exact numerical calculations for finite numbers of spins with $S=\frac{1}{2}$, chiefly for $N=200$, 500, 2000, 5000, and 20 000 spins. The results are remarkable for the unexpected width in temperature exhibited by the transition. The program was carried out for such high values of N because preliminary results for lower values showed a very poorly developed transition. We remark that for the uniform interaction (1) we can handle 20 000 spins with less difficulty than 10 spins coupled only by nearest-neighbor interactions, as in calculations by Orbach[2] and others.

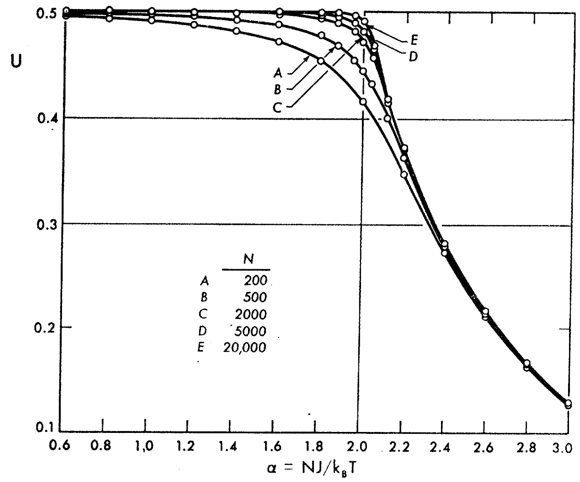

FIG. 2. Exchange energy U per spin as a function of the normalized reciprocal temperature. The curve is plotted for $NJ=2$.

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[2] R. Orbach, Phys. Rev. 112, 309 (1958).

Order Parameter Versus α

In Fig. 1 we present the results for the order parameter versus α, where $\alpha \equiv NJ/k_BT$. In an infinite system the transition occurs at $\alpha = 2$. The uppermost curve, labeled A, is for 200 spins; for this number of spins the variation of order with temperature is quite gradual. Only when we get to 20 000 spins, as in the lowermost curve labeled E, is the disorder reasonably well established in the high-temperature region, $\alpha < 2$. At low temperatures the differences in η for various N's are not pronounced.

The order parameter is calculated as

$$\langle\eta\rangle = 1 - 2\langle p\rangle/N = 1 - (2/NZ)\sum_p pG_p e^{-\lambda_p\beta}, \quad (20)$$

where the sum runs from $p=0$ to $p=\frac{1}{2}N$. Here Z is the partition function.

Internal Energy Versus α

In Fig. 2 we present the exchange energy U per spin as a function of α. The energy is calculated as

$$U = \frac{1}{NZ}\sum_p G_p \lambda_p e^{-\lambda_p\beta}. \quad (21)$$

For convenience the value $NJ = 2$ was taken.

Heat Capacity Versus α

In Fig. 3 the heat capacity C_v per spin is plotted as a function of α. The normalization of the heat capacity is given by the relation

$$C_v = -\beta^2(dU/d\beta), \quad (22)$$

and we have taken $NJ = 2$.

Entropy Versus α

In Fig. 4 the entropy σ per spin is plotted as a function of α. The entropy is given by

$$\sigma = -\beta^2(\partial F/\partial\beta), \quad (23)$$

where $F = (1/N\beta)\ln Z$.

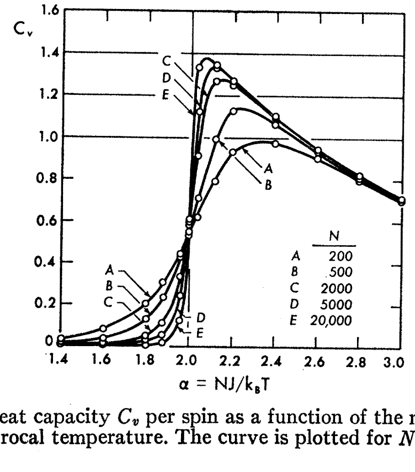

FIG. 3. Heat capacity C_v per spin as a function of the normalized reciprocal temperature. The curve is plotted for $NJ = 2$.

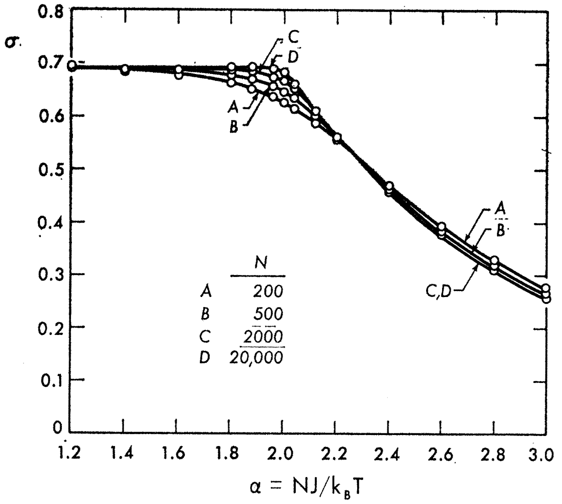

FIG. 4. Entropy σ per spin as a function of the normalized reciprocal temperature.

Magnetic Moment Versus α

In Fig. 5 we present the z component of the spin $\langle \mathbb{S}_z\rangle/N$ and also the value of $\langle \mathbb{S}\rangle/N$, both curves evaluated for a magnetic field $\mathcal{H}$ such that $g\mu_B\mathcal{H} = 0.1$; also, $NJ = 2$. The curves A refer to 50 spins. The differences between $\langle \mathbb{S}_z\rangle$ and $\langle \mathbb{S}\rangle$ are an effect of the superparamagnetic situation. The field $\mathcal{H}$ is quite strong and the transition would not be sharp even for an infinite system.

EXPLANATION OF BEHAVIOR OF SYSTEMS WITH FINITE NUMBER OF SPINS

We want to understand the slowness with which the transition develops as the number N of spins is increased. To do this we must retain several terms in the

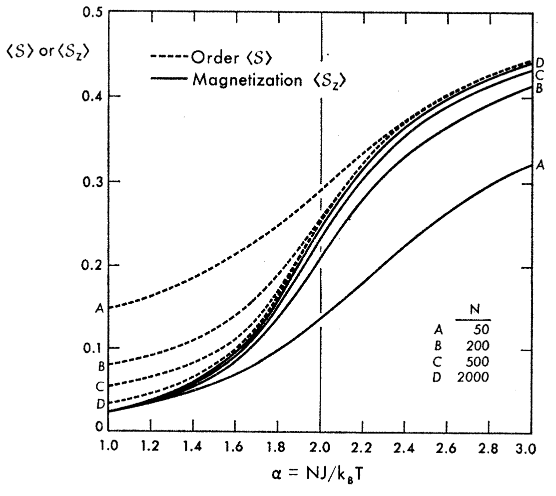

FIG. 5. Magnetic moment per spin and order versus α. Both are calculated for a magnetic field $\mathcal{H}$ such that $g\mu_B\mathcal{H} = 0.1$ and with $NJ = 2$.

partition function (5) which were neglected in the approximation (6), and then we must evaluate the partition function more carefully.

Let us consider the particular problem of finding the value of the order parameter $\eta \equiv 1-2p/N$ at the temperature $\alpha=2=NJ/k_BT$ which is, according to (11), the Curie temperature of the infinite system. At this temperature the exponent of the pth term of the partition function is

$$N\ln N-(N-p+1)\ln(N-p)-p\ln p+2\ln(N-2p) \\ -2p+2p^2/N+\tfrac{1}{2}\ln N-\tfrac{1}{2}\ln(N-p)-\tfrac{1}{2}\ln p, \quad (24)$$

where now we have taken the Stirling approximation as

$$x!\cong x^x e^{-x}(2\pi x)^{1/2}. \quad (25)$$

The term $(2\pi x)^{1/2}$ will turn out to have little importance. In (24) we have written $\ln(N-p)$ for $\ln(N-p+1)$ and dropped terms of the order of unity.

It is convenient to rewrite (24) in terms of η. If we put to one side terms which do not involve η we obtain

$$\tfrac{1}{2}N\{-\ln(1-\eta^2)-\eta\ln(1+\eta)/(1-\eta)+\eta^2\} \\ -\tfrac{3}{2}\ln(1+\eta)-\tfrac{1}{2}\ln(1-\eta)+2\ln\eta. \quad (26)$$

The extremum is given when the derivative of (26) with respect to η is zero:

$$N\eta-N\ln\frac{1+\eta}{1-\eta}+\frac{2\eta-1}{1+\eta^2}+\frac{2}{\eta}=0. \quad (27)$$

Equation (27) becomes, on expanding the ln,

$$-\tfrac{1}{3}N\eta^3+\frac{2\eta-1}{1+\eta^2}+\frac{2}{\eta}=0. \quad (28)$$

If we are concerned with N sufficiently large that η will be $\ll 1$ we may drop the term in $(2\eta-1)/(1+\eta^2)$ in (28), so that

$$\tfrac{1}{3}N\eta^3=2/\eta, \quad (29)$$

whence the most probable value of η at the Curie temperature given by

$$\eta_{\text{mp}}=(6/N)^{1/4}=1.56/N^{1/4}. \quad (30)$$

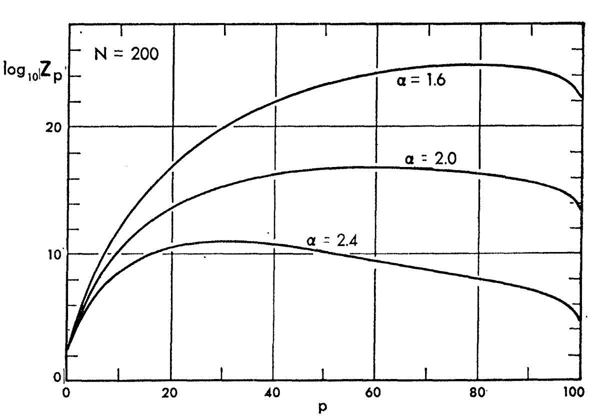

FIG. 6. The $\log_{10}$ of the individual contributions to the partition function, for 200 spins and for three values of the normalized reciprocal temperature. The nominal Curie temperature is at $\alpha=2.0$. No magnetic field is present. Here $\alpha=NJ/k_BT$.

Notice that it is the fourth root and not the square root of N which enters. For $N=10\,000$, we have $\eta_{\text{mp}}\cong 0.16$; for $N=100$, we have $\eta_{\text{mp}}\approx 0.5$. It takes a large system to obtain a low value of the order at the nominal Curie temperature.

From (29) we see that the leading η-dependent parts of (25) are the terms

$$-\tfrac{1}{12}N\eta^4+2\ln\eta, \quad (31)$$

so that the argument of the partition function at small η is proportional to

$$\eta^2 e^{-N\eta^4/12}. \quad (32)$$

Thus, the *mean value* $\langle\eta\rangle$ of η at the transition temperature is given approximately by

$$\langle\eta\rangle=\int_0^\infty d\eta\,\eta^3 e^{-N\eta^4/12}\bigg/\int_0^\infty d\eta\,\eta^2 e^{-N\eta^4/12}=\frac{(12)^{1/4}}{\Gamma(\frac{3}{4})N^{1/4}} \quad (33)$$

or

$$\langle\eta\rangle=1.52/N^{1/4}. \quad (34)$$

We notice that for finite N the mean value (34) is not identical with the most probable value (30). The difference is

$$\eta_{\text{mp}}-\langle\eta\rangle\cong 0.04/N^{1/4}. \quad (35)$$

The contributions to the partition function at the nominal Curie temperature are plotted in Fig. 6. Here Z_p is an individual term in the partition function (5); that is, $Z=\sum_p Z_p$. Notice how flat the maximum is, even allowing for the logarithmic scale. The difference (35) is the result of the poor definition shown by the curve.

SELF-CONSISTENT APPROXIMATION

We reconsider our exact solution (9) for ferromagnetic spin order in the light of the approximation method developed by Bloch[3] and applied by her to problems with nearest-neighbor interactions. It is simple to adapt her method to the uniform interaction which concerns us here. If we neglect the uniform mode, we have to deal with N oscillators of frequency ϵ_0 $(=NJ)$ in the absence of magnon interactions. In the self-consistent (Bloch) approximation the ensemble average occupancy of each oscillator is

$$\langle n\rangle=1/(e^{\beta\epsilon(T)}-1), \quad (36)$$

where the renormalized oscillator is

$$\epsilon(T)=\epsilon_0(1-2\langle n\rangle). \quad (37)$$

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[3] M. Bloch, Phys. Rev. Letters **9**, 286 (1962); J. Appl. Phys. **34**, 1151 (1963).

This result follows from our exact eigenvalue equation, (3). In terms of the usual order parameter

$$\eta=1-2\langle n\rangle, \tag{38}$$

we have

$$\tfrac{1}{2}(1-\eta)=1/(e^{\beta\epsilon_0\eta}-1), \tag{39}$$

or

$$\ln[(3-\eta)/(1-\eta)]=\beta\epsilon_0\eta, \tag{40}$$

which may be compared with the exact result

$$\ln[(1+\eta)/(1-\eta)]=\beta\epsilon_0\eta, \tag{41}$$

obtained earlier as Eq. (9). Solutions of these two equations are compared in Fig. 7.

It may be noted that the use of a fermion distribution in place of (36) for $\langle n\rangle$ will lead to the correct result (41). Hopfield (private communication) has proposed an ingenious explanation of this, which will be developed by one of us (H.S.) in his thesis.

The inadequacy of the self-consistent approximation here is quite unexpected, as it appears to be remarkably good for nearest-neighbor interactions. In all instances, however, the approximation leads to double-valued results. Because our expression for $\epsilon(T)$ is exact in the present problem, it is evident that the statistics are responsible for the difficulties, and not the energy. The introduction of a chemical potential into the boson distribution function has been examined by us, but this does not appear to improve the situation.

ANTIFERROMAGNETIC GROUND STATE

The true antiferromagnetic ground state is also the highest energy state of the Hamiltonian $H'=-J\mathbb{S}\cdot\mathbb{S}$ for positive J. How good an approximation to the highest energy state is the alternating spin function

$$\psi_a=\alpha_1\beta_2\alpha_3\beta_4\cdots\alpha_{N-1}\beta_N? \tag{42}$$

This state is called the Néel state. The true maximum energy of H' for even N is just zero, for $\mathbb{S}_{\min}=0$.

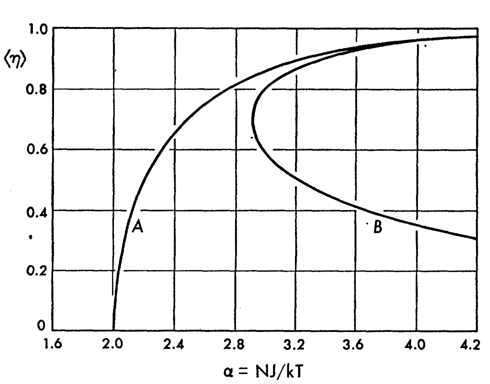

FIG. 7. Order parameter η as a function of the normalized reciprocal temperature, for an infinite system. Curve A is for the exact solution, Eq. (9); curve B is for the self-consistent approximation.

Now the expectation value of H' for ψ_a is given by

$$\langle\psi_a|-J\sum_{i\neq j}\mathbf{S}_i\cdot\mathbf{S}_j-J\sum_i S_i^2|\psi_a\rangle$$

$$=-\tfrac{1}{4}NJ[(\tfrac{1}{2}N-1)-\tfrac{1}{2}N]-\tfrac{3}{4}NJ=-\tfrac{1}{2}NJ, \tag{43}$$

which is exceedingly close to the correct energy because NJ is only of the order of k_BT_C.

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APPENDIX A: MEAN VALUES ON THE MOLECULAR-FIELD MODEL

For the molecular-field model at the nominal Curie temperature $\alpha=2$ we have

$$Z_I=\sum_0^N\frac{N!}{(N-r)!r!}e^{-2r+2r^2/N}. \tag{A1}$$

With (25) as the Stirling approximation the condition for the extremum of the terms of the partition function is

$$N\ln\frac{1+\eta}{1-\eta}-2N\eta-\frac{2\eta}{1-\eta^2}=0. \tag{A2}$$

After expanding the ln we have

$$\tfrac{2}{3}N\eta^3\cong2\eta, \tag{A3}$$

so that the most probable value of η is given by

$$\eta_{\mathrm{mp}}=(3/N)^{1/2}. \tag{A4}$$

Notice that this involves $N^{-1/2}$ and not $N^{-1/4}$. The *mean value* of η on this model is given by

$$\langle\eta\rangle\cong\int_0^\infty d\eta\eta e^{-N\eta^4/12}\Big/\int_0^\infty d\eta e^{-N\eta^4/12}$$

$$=(12/N)^{1/4}\Gamma(\tfrac{1}{2})/\Gamma(\tfrac{1}{4})\cong0.91/N^{1/4}. \tag{A5}$$

This is different from the most probable value of η even in the dependence on N.

The common assumption in statistical mechanics that mean values of variables are closely equal to their most probable values is seen to be poorly satisfied by the molecular-field model, except for extremely large numbers of particles.