Rejoinder on "Conjectures on exact solution of three-dimensional (3D) simple orthorhombic Ising lattices"[*]

Jacques H.H. Perk[†]

145 Physical Sciences, Oklahoma State University,
Stillwater, OK 74078-3072, USA[‡]
and
Department of Theoretical Physics, (RSPE), and
Centre for Mathematics and its Applications (CMA),
Australian National University,
Canberra, ACT 2600, Australia

March 30, 2009

Abstract

It is shown that the arguments in the reply of Z.-D. Zhang defending his conjectures are invalid. His conjectures have been thoroughly disproved.

After all the discussion about his paper [1, 2, 3, 4, 5], Zhang seems to have only one real issue left with the two comments [2, 5], still wrongly believing [6] that the free energy of the three-dimensional Ising model is not analytic at $\beta \equiv 1/(k_{\rm B}T) = 0$, $H = 0$. His further arguments are irrelevant or dealt with adequately in [2, 5].

[*]Supported by NSF grantPHY 07-58139
[†]Email: perk@okstate.edu
[‡]Permanent address

His objection that Gallavotti and Miracle-Solé set $\beta = 1$ is not valid. One often uses dimensionless parameters $K_i = \beta J_i$, $(i = 1, 2, 3)$, $h = \beta H$. Equivalently, one can absorb the β into the coupling constants, setting $\beta = 1$, so that $K_i \equiv J_i$, $h \equiv H$. Infinite temperature is then the limit $K_i \to 0$, $h \to 0$, such that all ratios are kept fixed.[1]

His point on [7] is also not valid. Writing $z \equiv \exp(-2\beta H)$, see eq. (23) of [7], and keeping βH fixed in the limit $\beta \to 0$, the Ising model partition function on an arbitrary lattice with N sites becomes $Z = (z^{1/2} + z^{-1/2})^N$, so that all infinite-temperature zeros of Z occur at $z = -1$, i.e. for the purely imaginary magnetic field [7] $H = \pm i\pi k_{\mathrm{B}}T/2 = \pm i\infty$. There is no $T = \infty$ singularity at $H = 0$, $z = 1$.[2]

References

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[1] The reduced free energy per site βf is often rewritten $\beta f = \phi(\{K_i\}, h) = \phi(\{\beta J_i\}, \beta H)$ with some function ϕ. Setting $\beta = 1$ is no loss of generality, as one can easily restore the β-dependence by the replacements $J_i \to \beta J_i$, $H \to \beta H$, $f \to \beta f$.

[2] In Zhang's paper [1], $H \equiv 0$, $z \equiv 1$, $Z = 2^N$ for any lattice with N sites at $T = \infty$, which is far from $z = -1$. Hence, the infinite-system dimensionless free energy βf is analytic at $\beta = 0$ also by the general theory of Yang and Lee [8].

Added Comments

It has saddened my heart to see arXiv:0812.0194v3 and to see that Zhang is still not convinced that his conjectured results are in error. For his benefit and the benefit of others who might be confused by his remarks I am adding the following to show why his newer statements are also in error.

The probability interpretation of statistical mechanics involves Z and thus βf. Therefore, that $f \to \infty$ for the free energy per site as $T \to \infty$ is of no physical significance. Series and analyticity determinations must be starting from the reduced free energy $\beta f = f/k_{\rm B}T$, not f, near $T = \infty$.

Also, as long as (the real part of) f is negative, (which is easily checked for the Ising model at arbitrary temperature), $Z = \exp(-N\beta f)$ blows up and $1/Z \to 0$ as $N \to \infty$. So $\lim_{N\to\infty} 1/Z = 0$ occurs for all finite temperatures even at the critical point where the Yang–Lee zeroes pinch the real axis. It is a misinterpretation of the Yang–Lee papers to study zeroes of $1/Z$. The Boltzmann probability is given by $\exp(-\beta\mathcal{E})/Z$, with Z a polynomial in $z = \exp(-2\beta H)$, H being the scaled magnetic field. This probability can only show anomalous behavior if zeroes of Z approach as $N \to \infty$, as is clearly explained by Yang and Lee in their two famous 1952 papers.

Finally, there are many papers proving analyticity of the reduced free energy in $1/T$ around $T = \infty$, for both classical and quantum models that generalize the Ising model. Such proofs have been published by many groups in Europe, Russia, Japan and America. I have only quoted a few mostly Ising references in my comment. The exactness of the series is rigorously proved many times. It is also backed up by numerical work, as Padé analysis of the series expansion is in excellent agreement with other numerical work, such as Monte Carlo calculations. There can be no such evidence backing up Zhang's work, as it violates rigorously established theorems.

Added Comments 2

As Zhang is stacking up further errors in his fourth version arXiv:0812.0194v4 and repeats his errors to the followers of his blog in China, I feel that I have little choice than adding another reply.

In the first place, under "solving the three-dimensional Ising model" is understood the calculation of some basic thermodynamic quantities using standard equilibrium statistical mechanics starting from $\hat{H}$ in [1], i.e. the usual Ising interaction energy. Any talk about time dependence, ergodicity, relativity, quantum mechanics, black holes, etc., is a distraction from the well-defined problem and changing it to a different problem.

Standard equilibrium statistical mechanics states that the free energy per site f is calculated using

$$\beta f = \frac{1}{N}\beta F = -\frac{1}{N}\log Z, \tag{1}$$

with Z the partition function and N the number of sites. It is βf which is calculated first and it is βf for which series expansions are done. That f becomes ∞ at $T = \infty$ is of no significance, as is obvious from one of the basic formulae in thermodynamics, $F = U - TS$. This says that at $T = 0$ we have $F = U$ the (internal) energy, while at $T = \infty$ we find $F/T = -S$, i.e. minus the entropy. This explains again that F/T, or equivalently βF, is preferred over F at high temperatures.

Next, consider eq. (1) in Zhang's paper [1], and define

$$C = \max\{|J|, |J'|, |J''|\}, \tag{2}$$

the absolute maximum of the coupling constants. Then it is easily checked that

$$|\hat{H}| \le 3NC, \quad |Z| \le 2^N e^{3NC}, \quad \frac{1}{N}\log|Z| \le \log 2 + 3C, \tag{3}$$

as the number of terms in Z is 2^N. The only way to get singularities in βf is the occurrence of zeroes of Z, as explained excellently by Yang and Lee, whom Zhang chooses to misquote. Zhang's work is in stark contradiction with the work of Yang and Lee as a result.

Finally, using the logic of his conjecture we can solve almost any problem in statistical mechanics, but with incorrect results. The idea of going to higher dimension is a generalization of the fundamental theorem of calculus $\int_a^b f'(x)\mathrm{d}x = f(b) - f(a)$, with examples the theorems of Green, Stokes, Gauss, and the Wess–Zumino term. For the "guess" to work, Zhang must show that the integrand in four dimensions is a derivative of the integrand in 3D (or a discrete version with integrand replaced by summand and derivative by some kind of difference). In [1] I cannot find that Zhang understands this and, as the conjecture is rigorously proved to be false, it makes no sense to further discuss this matter here.

Added Comments 3

Most proofs of the analyticity of free energies and correlation functions use linear correlation identities of Schwinger–Dyson type, known under such names as the BBGKY hierarchy, Mayer–Montroll or Kirkwood–Salzburg equations. If Zhang had read [9] in detail and understood, he would have found more than one way to arrive at a proof of analyticity of βf at $\beta = 0$. He would also have found [10] (ref. [12] cited in [9]). Let me try to explain the proof in more down-to-earth terms using an identity of Suzuki [11, 12], restricted to the isotropic Ising model on a simple cubic lattice with periodic boundary conditions and of arbitrary size, i.e.

$$\Big\langle \prod_{i=1}^{n} \sigma_{j_i} \Big\rangle = \frac{1}{n} \sum_{k=1}^{n} \Big\langle \Big(\prod_{\substack{i=1 \\ i \neq k}}^{n} \sigma_{j_i} \Big) \tanh \Big(\beta J \sum_{l \text{ nn of } j_k} \sigma_l \Big) \Big\rangle, \tag{4}$$

where $j_1, \ldots, j_n$ are the labels of n spins and l runs through the labels of the six spins that are nearest neighbors of σ_{j_k}. The isotropy assumption, i.e. $J_1 = J_2 = J_3 = J$, is made to simplify the argument, but can be easily lifted. Averaging over k has been added in (4), so that all spins are treated equally.

Next we use

$$\tanh \Big(\beta J \sum_{l=1}^{6} \sigma_l \Big) = a_1 \sum_{(6)} \sigma_l + a_3 \sum_{(20)} \sigma_{l_1}\sigma_{l_2}\sigma_{l_3} + a_5 \sum_{(6)} \sigma_{l_1}\sigma_{l_2}\sigma_{l_3}\sigma_{l_4}\sigma_{l_5}, \tag{5}$$

where the sums are over the 6, 20, or 6 choices of choosing 1, 3, or 5 spins from the given $\sigma_1, \ldots, \sigma_6$. It is easy to check that the coefficients a_i are

$$a_1 = \frac{t(1 + 16t^2 + 46t^4 + 16t^6 + t^8)}{(1+t^2)(1+6t^2+t^4)(1+14t^2+t^4)}, \quad a_3 = \frac{-2t^3}{(1+t^2)(1+14t^2+t^4)},$$
$$a_5 = \frac{16t^5}{(1+t^2)(1+6t^2+t^4)(1+14t^2+t^4)}, \quad t \equiv \tanh(\beta J). \tag{6}$$

The poles of the a_i are at $t = \pm \mathrm{i}$, $t = \pm(\sqrt{2} \pm 1)\mathrm{i}$, and $t = \pm(\sqrt{3} \pm 2)\mathrm{i}$. It can also be verified, e.g. expanding the a_i in partial fractions, that the series expansions of the a_i in terms of the odd powers of t alternate in sign and converge absolutely as long as $|\beta J| < \arctan(2 - \sqrt{3}) = \pi/12$.

The system of equations (4)–(6) can be viewed as a linear operator on the vector space of all correlation functions of the 3d Ising model. It is easy to estimate the norm of this operator, from the $32n$ terms in the right-hand side (RHS) of (4) after applying (5), using the alternating sign property of the a_i's. It follows that we only need to study

$$6a_1 + 20a_3 + 6a_5 = \frac{2t(t^2+3)(3t^2+1)}{(1+t^2)(1+14t^2+t^4)} \qquad (7)$$

for purely imaginary t to find the desired upper bound r for the norm. We then have that the RHS of (4) is bounded by rM, where $M = \max|\langle\sigma\cdots\sigma\rangle|$ with the maximum taken over all $32n$ pair correlations in the RHS. Obviously, $M \leq 1$ if $\beta \geq 0$ and real. We must stress that the bound is also valid if all the a_i's are replaced by the power series in t obtained from the power series of the a_i's replacing each term by its absolute value.

According to the above we set r equal to the absolute value of (7) for imaginary t. We can then show that $r < 1$ for

$$\begin{aligned} &|t| < (\sqrt{3}-\sqrt{2})(\sqrt{2}-1) = 0.131652497\cdots, \quad \text{or} \\ &|\beta J| < \arctan[(\sqrt{3}-\sqrt{2})(\sqrt{2}-1)] = 0.130899693\cdots. \end{aligned} \qquad (8)$$

To prove analyticity of βf in terms of β at $\beta = 0$ it suffices to study the internal energy per site or the nearest-neighbor pair correlation function, as

$$u = \frac{\partial(\beta f)}{\partial \beta} = -3J\langle\sigma_{000}\sigma_{100}\rangle. \qquad (9)$$

We apply (4) to $\langle\sigma_{000}\sigma_{100}\rangle$, then we apply (4) on each of the new correlations, and we keep repeating this process. We may now and then encounter a correlation with zero σ factors $\langle 1\rangle = 1$, at which the process ends. As each other correlation vanishes with a power of t, we then generate the high-temperature power series to higher and higher orders, for arbitrary given size of the system. The series is absolutely convergent as the sum of the absolute values is bounded by $\sum r^j < \infty$ when (8) holds. We can at first assume that $\beta \geq 0$ and real. But from the absolute convergence we also obtain a finite radius of convergence in the complex t and β planes.

Increasing the size of the system, we conclude that more and more terms become independent of the size, whereas the remainder rapidly tends to zero. Therefore, the series converges to the thermodynamic limit, and we have once again proved that the free energy and all correlation functions are analytic in t and in β, as long as (8) holds. This bound is a rough estimate and much better ones have been given in the literature. Furthermore, adding a small magnetic field H and generalizing the steps in the above, we can also conclude that all correlation functions are finite for small enough β and H, so that there are no Yang–Lee zeroes near the $H = 0$ axis for small β.

In conclusion once more, papers [1, 3, 6] contain serious errors and are beyond repair.

References

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