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COMMENT

Comments on ferroelectric ice model on a triangular lattice†

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Abstract. It is shown that the free energy per vertex for a ferroelectric ice model on a triangular lattice can be expressed in terms of elementary functions. An exact upper bound for the residual entropy of ice on a Kagomé lattice is obtained.

Kelland (1974a) solved exactly a ferroelectric ice model on a triangular lattice. The free energy per vertex \mathcal{F} is given by the principal value integral (we follow the notation of Kelland)

$$-\beta\mathcal{F} = P \int_{-\infty}^{\infty} \frac{16 \sinh(\pi - \phi)m \cosh^3(\pi - \phi)m}{m(e^{2\phi m} + 1)(1 - e^{-2\pi m})} dm \tag{1}$$

where

$$2 \cos \phi = -\sqrt{1 + u^{-1}} \quad \frac{2}{3}\pi < \phi < \pi.$$

The integral (1) was later integrated by Kelland to give (Kelland 1974b, equations (57) and (58))

$$-\beta\mathcal{F} = 2 \int_{-\infty}^{\infty} \frac{\sinh^2(\pi - \phi)m \cosh^3(\pi - \phi)m}{m \cosh(\phi m) \sinh(\pi m)} dm \tag{2}$$

$$= - \sum_{m=1}^{\infty} \frac{2}{m} \sin^2(2m\phi) + \sum_{m=1}^{\infty} \frac{4}{2m-1} \sin^2[(2m-1)\pi^2/\phi]. \tag{3}$$

It is interesting to note that Kelland's expression (3) can be evaluated in terms of elementary functions as follows:

$$-\beta\mathcal{F} = \lim_{N \rightarrow \infty} \left(- \sum_{m=1}^N \frac{2}{m} \sin^2(2m\phi) + \sum_{m=1,2,\dots} \frac{4}{2m-1} \sin^2[(2m-1)\pi^2/\phi] \right)$$

$2m-1 < 2\phi N/\pi$

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and so

$$\begin{aligned}
 -\beta\mathcal{F} &= \lim_{N \rightarrow \infty} \left(-\sum_{m=1}^N \frac{1}{m} + \sum_{m < \phi N / \pi} \frac{2}{2m-1} \right) \\
 &\quad + \sum_{m=1}^{\infty} \frac{\cos(4\phi m)}{m} - \sum_{m=1}^{\infty} \frac{2}{2m-1} \cos\left(\frac{(2m-1)2\pi^2}{\phi}\right) \\
 &= \ln\left(\left|\frac{2\phi \tan(\pi^2/\phi)}{\pi \sin(2\phi)}\right|\right). \tag{4}
 \end{aligned}$$

In particular, the case $u = 1$ corresponds to the triangular ice model of Baxter (1969) and $-\beta\mathcal{F} = \ln W$ where $W = 3\sqrt{3}/2 = 2.598 \dots$

Recently it has been shown by Lin (1976) that the ice model on a Kagomé lattice (Lin and Tang 1976) is equivalent to a special case of the 20-vertex model on a triangular lattice such that (in the notation of Kelland)

$$u_1 = u_2 = u_3 = u_5 = u_8 = u_9 = 1 \quad u_4 = u_6 = u_7 = u_{10} = 2. \tag{5}$$

Since the soluble condition (Kelland 1974b, equation (19)) is not satisfied, the residual entropy of ice on a Kagomé lattice cannot be obtained by the method of Bethe *ansatz*. Instead we have an exact upper bound for the ice model on a Kagomé lattice:

$$W(\text{Kagomé lattice}) < (e^{-\beta\mathcal{F}/3})_{u=2} = 1.708 \dots \tag{6}$$

This upper bound is an improvement on that obtained by Lin (1976) of $3^{1/2} = 1.732 \dots$

References

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