High-temperature series for the spin-one Ising model for arbitrary biquadratic exchange, field, and anisotropy

R. I. Joseph
Department of Electrical Engineering, The Johns Hopkins University, Baltimore, Maryland 21218

R. A. Farrell*
Applied Physics Laboratory, The Johns Hopkins University, Laurel, Maryland 20810

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The spin-one Ising system $-\beta\mathcal{H} = K\sum_{\langle i,j\rangle}(S_iS_j + \eta S_i^2S_j^2) + \sum_k (hS_k + \Lambda S_k^2)$ is considered. We have obtained high-temperature series for the free energy through eighth order for arbitrary η, h, and Λ by rewriting this Hamiltonian in a form which exploits its relation to the three-component Potts model ($\eta = 3$). Explicit results are presented for the bcc lattice.

The Blume-Emery-Griffiths model[1] is a spin-one Ising system characterized by the Hamiltonian

$$-\beta\mathcal{H}=K\sum_{\langle i,j\rangle}(S_iS_j+\eta S_i^2S_j^2)+\sum_{k=1}^{N}\zeta_k(h,\Lambda);\qquad \zeta_k(h,\Lambda)=hS_k+\Lambda S_k^2. \tag{1}$$

Blume *et al.*[1] studied Eq. (1) in the mean-field approximation to elucidate the λ transition and phase separation in ^{3}He-^{4}He. Dunn and Essam[2] have shown that a decorated spin-one Ising model can be reduced to the form of Eq. (1). Additional situations where the model has applicability are discussed in the review paper of Nagle and Bonner.[3] For $\eta \gg 1$ and $h=0$, the system is equivalent to a spin-$\frac{1}{2}$ Ising model in a temperature-dependent field.[4] When $\eta=3$, it reduces to the three-component Potts model for which eighth-order high-temperature series for arbitrary h and Λ are known on the Bravais lattices.[5] If $\eta=1$, similar results are straightforward to obtain. Ditzian and Oitmaa[6] have obtained sixth-order high-temperature series for $h=0$ with η, Λ arbitrary on the fcc lattice.

In the present paper, we show that by utilizing the functional form of the appropriate Potts-model interaction,

$$\delta_{S_iS_j}=\tfrac{1}{2}S_iS_j+\tfrac{3}{2}S_i^2S_j^2-(S_i^2+S_j^2)+1, \tag{2}$$

Ref. 7, Eq. (1) can be cast into a form which reduces considerably the labor of calculating high-temperature series coefficients for arbitrary η, h, and Λ. In fact, through fifth order for Bravais lattices the series coefficients can be simply read off from those available for the Potts model.[5] On the loose-packed lattices, this is even true through seventh order and in the eighth order, the additional computations that are necessary are quite modest.

Now since $S_i^3=S_i$, it follows directly from Eq. (2) that we can write

$$2S_iS_j\delta_{S_iS_j}=S_iS_j+S_i^2S_j^2;\quad (1-S_iS_j)\delta_{S_iS_j}=S_i^2S_j^2-(S_i^2+S_j^2)+1. \tag{3}$$

Hence, Eq. (1) can be rewritten in the equivalent form

$$-\beta\mathcal{H}=K\sum_{\langle i,j\rangle}[2S_iS_j+(\eta-1)(1-S_iS_j)]\delta_{S_iS_j}+\sum_k\zeta_k(h,\Lambda')-\tfrac{1}{2}NzK(\eta-1), \tag{4}$$

where $\Lambda'\equiv\Lambda+Kz(\eta-1)$ and z is the lattice coordination number. Using the identity $e^{ax}\equiv 1+x(e^a-1)$ if $x=0,1$, the partition function Z for Eq. (4) takes the form

$$Z=e^{-NzK(\eta-1)/2}\,\mathrm{tr}\prod_{\langle i,j\rangle}\{1+\delta_{S_iS_j}[uS_iS_j+v(1-S_iS_j)]\}\exp\left(\sum_k\zeta_k(h,\Lambda')\right), \tag{5}$$

with $u\equiv e^{2K}-1$, $v\equiv e^{K(\eta-1)}-1$, and where we have used the fact that $S_iS_j(1-S_iS_j)\delta_{S_iS_j}=0$ in order to eliminate the uv term. For convenience, we now let

$$
\begin{aligned}
g &\equiv \sum_{S_k=0,\pm 1} e^{\zeta_k(h,\Lambda')} = 1 + 2e^{\Lambda'}\cosh h, \\
g(m,l) &\equiv \sum_{S_k=0,\pm 1} [uS_k^2 + v(1-S_k^2)]^l e^{m\zeta_k(h,\Lambda')} \\
&= v^l + u^l(2e^{m\Lambda'}\cosh mh), \\
G(m,l) &\equiv g(m,l)/g^m.
\end{aligned} \tag{6}
$$

For the Potts model $(\eta = 3), u = v$. The $G(m,l)$ are then of the form $u^l G_m$. One then evaluates Z by expanding the right-hand side of Eq. (5) in powers of u. The first term is g^N and each l-line graph which can be drawn on a lattice contributes to the lth power of u with a factor determined by the topology of the graph. Factoring out g^N, an m-vertices-connected graph gives a factor G_m so each u^l coefficient will be a linear combination of terms of the form $G_2^{\alpha_2} G_3^{\alpha_3} \cdots$. This simplification is due to the factor $\delta_{S_i S_j}$ associated with each line in the graph. In the thermodynamic limit the free energy per particle f then takes the form

$$
-\beta f = -zK + \ln g + \sum_{l=1}^{\infty} \frac{u^l}{l!} F_l(G), \tag{7}
$$

where $F_1 = \frac{1}{2} z G_2$, $F_2 = z(z-1)G_3 - z(z-\frac{1}{2})G_2^2, \ldots$, and $\eta = 3$ is used. $F_1 - F_8$ have been explicitly obtained on the Bravais lattices by Kim and Joseph.[5] Each term appearing in a given F_l comes from a distinct topological set of graphs which contribute similarly because of the $\delta_{S_i S_j}$ factor. For arbitrary η, we could expand in a double power series in u, v. However, it is not necessary to carry this out in detail. Consider a term $u^l G_{q_1}^{\alpha_1} G_{q_2}^{\alpha_2} \cdots$ appearing in Eq. (7) and the expression $[G(q_1, p_1)]^{\alpha_1} \times [G(q_2, p_2)]^{\alpha_2} \cdots$, where $\alpha_1 p_1 + \alpha_2 p_2 + \cdots = l$. If there is a unique set $p_1, p_2 \ldots$ satisfying this condition, then the result for arbitrary η can be directly written down from the $\eta = 3$ result by the replacement

$$
u^l G_{q_1}^{\alpha_1} G_{q_2}^{\alpha_2} \cdots \to [G(q_1, p_1)]^{\alpha_1} [G(q_2, p_2)]^{\alpha_2} \cdots .
$$

If there is not a unique set of $p_1, p_2, \ldots$, recalculation is required. This procedure is simplified by noting that q_i specifies the number of vertices in a connected graph and the quantity p_i gives the number of lines in the graph so that these numbers must obey the restrictions that $\frac{1}{2} q_i (q_i - 1) \geq p_i \geq q_i - 1$. Thus, for example, $u^2 G_3$ is uniquely replaced by $G(3, 2)$. Similarly $u^2 G_2^2 \to [G(2,1)]^2$. Going through the known term structure factors for the Potts model[5] (there are 1, 2, 4, 7, 12, 21, 32, 50 terms for $l = 1, \ldots, 8$, respectively), we find that through fifth order this replacement is uniquely defined. In sixth order, this can be done for all terms but the single term $u^6 G_3 G_4$. There are two distinct sets of graphs which contribute to the latter term, and the factors associated with these graphs are $G(3,3)G(4,3)$ and $G(3,2)G(4,4)$. Similarly in seventh order, there are three terms for which we cannot uniquely make the replacement: $u^7 G_3 G_5 \to G(3,2)G(5,5),\ G(3,3)G(5,4)$; $u^7 G_2 G_3 G_4 \to G(2,1)G(3,2)G(4,4),\ G(2,1)G(3,3)G(4,3)$; $u^7 G_3 G_4 \to G(3,2)G(4,5),\ G(3,3)G(4,4)$. In eighth order there are seven terms:

$$
\begin{aligned}
&u^8 G_3 G_6 \to G(3,2)G(6,6),\ G(3,3)G(6,5); \\
&u^8 G_4 G_5 \to G(4,3)G(5,5),\ G(4,4)G(5,4); \\
&u^8 G_2 G_3 G_5 \to G(2,1)G(3,2)G(5,5),\ G(2,1)G(3,3)G(5,4); \\
&u^8 G_3 G_5 \to G(3,2)G(5,6),\ G(3,3)G(5,5); \\
&u^8 G_2^2 G_3 G_4 \to [G(2,1)]^2 \\
&\qquad \times G(3,2)G(4,4),\ [G(2,1)]^2 G(3,3)G(4,3); \\
&u^8 G_2 G_3 G_4 \to G(2,1)G(3,2)G(4,5),\ G(2,1)G(3,3)G(4,4); \\
&u^8 G_3 G_4 \to G(3,2)G(4,6),\ G(3,3)G(4,5).
\end{aligned}
$$

All of these terms arise from disconnected graphs. Hence for arbitrary η one has to recalculate the separate contributions of each set of graphs which make up the two possible factors. Their sum is of course just the factor occurring for the Potts model. At this point, in order to simplify our considerations, we shall restrict our attention to the loose-packed lattices. The reason for doing this is simply that certain kinds of graphs cannot be found on these lattices, and in particular no triangular configurations can occur [terms with the factor $G(3,3)$ do not contribute]. Taking this into account, we find that the nonuniqueness in the replacements in all remaining sixth- and seventh-order terms disappears as well as for all remaining eighth-order terms except for those arising from $u^8 G_4 G_5$. Hence to obtain eighth-order series for arbitrary η on loose-packed lattices, the only recalculation necessary is to find the individual contributions of graphs of the form $G(4,3)G(5,5)$ and $G(4,4)G(5,4)$. This is straightforward. The lattice constant of a disconnected graph can be expressed in terms of those of connected ones and these in turn are directly obtained from Baker *et al.*[8] Hence with a rather modest amount of additional work we have been able to obtain eighth-order series for the plane square, sc, and bcc lattices. In accord with Eq. (7), we shall write the free energy in the form

$$
-\beta f = -\tfrac{1}{2} zK(\eta - 1) + \ln g + \sum_{n=1}^{\infty} \frac{\hat{F}_n}{n!}. \tag{8}
$$

Explicit results for $\hat{F}_1 - \hat{F}_8$ on the bcc lattice are given in our Appendix.[9]

Finally, we point out that the present results also apply directly to the more general spin-one Ising system which would result from including the term $\frac{1}{2}\sigma S_i S_j (S_i + S_j)$ in Eq. (1) in addition to the term $\eta S_i^2 S_j^2$. Since $S_i S_j (S_i + S_j) \equiv (S_i + S_j)\delta_{S_i S_j}$, one can show that the free-energy expansion for this situation is obtained by replacing the $g(m,l)$ of Eq. (6) by the more general structures

$$g(m,l) = v^l + e^{m\Delta'}\{e^{mh}[u + (u+1)(e^{\sigma K} - 1)]^l + e^{-mh}[u + (u+1)(e^{-\sigma K} - 1)]^l\}. \quad (9)$$

In addition to the special cases $\sigma = 0$ with $\eta = 3$ (Potts model) or $\eta = 1$, this expression also simplifies for the cases $\sigma = \pm 2$ with $\eta = 1$ or $\eta = 5$ so that series results can be immediately obtained from those for the Potts model.

APPENDIX

Coefficients $\hat{F}_n$ for the bcc lattice [see Eq. (8)]. The following abbreviated notation is used: $R_k \equiv G(k, k-1)$, $S_k \equiv G(k,k)$, $T_k \equiv G(k, k+1)$, $U_k \equiv G(k, k+2)$.

$$\hat{F}_1 = 4R_2.$$

$$\hat{F}_2 = 56R_3 - 60R_2^2.$$

$$\hat{F}_3 = 1512R_4 - 3696\,R_2R_3 + 2192\,R_2^3.$$

$$\hat{F}_4 = 61\,680R_5 - 174\,240R_2R_4 - 74\,688R_3^2 + 319\,392R_2^2R_3 - 132\,456R_2^4 + 288\,S_4.$$

$$\hat{F}_5 = 3\,403\,200R_6 - 10\,964\,160R_2R_5 - 8\,706\,240R_3R_4 + 21\,693\,600R_2^2R_4 + 18\,639\,360R_2R_3^2 - 35\,373\,120R_2^3R_3 + 11\,313\,216R_2^5 + 34\,560S_5 - 40\,320R_2S_4.$$

$$\hat{F}_6/120 = 1\,979\,352R_7 - 7\,186\,272R_2R_6 - 5\,432\,160R_3R_5 + 15\,453\,912R_2^2R_5 - 2\,516\,724R_4^2 + 24\,602\,976R_2R_3R_4 + 3\,522\,632R_3^3 - 26\,240\,688R_2^3R_4 - 33\,871\,824R_2^2R_3^2 + 40\,150\,080R_2^4R_3 - 10\,462\,752R_2^6 + 32\,208\,S_6 - 60\,048R_2S_5 - 19\,944R_3S_4 + 49\,176R_2^2S_4 + 72T_5.$$

$$\hat{F}_7/120 = 167\,424\,264R_8 - 677\,169\,360R_2R_7 - 495\,122\,880R_3R_6 + 1\,582\,899\,696R_2^2R_6 - 436\,968\,000R_4R_5 + 2\,399\,627\,664R_2R_3R_5 + 1\,112\,243\,328R_2R_4^2 - 2\,841\,235\,488R_2^3R_5 + 955\,273\,536R_3^2R_4 - 6\,797\,917\,728R_2^2R_3R_4 - 1\,949\,474\,016R_2R_3^3 + 4\,428\,268\,992R_2^4R_4 + 7\,630\,367\,472R_2^3R_3^2 - 6\,510\,434\,112R_2^5R_3 + 1\,432\,274\,112R_2^7 + 3\,797\,136S_7 - 9\,328\,032R_2S_6 - 4\,125\,744R_3S_5 + 11\,640\,384R_2^2S_5 - 1\,604\,736R_4S_4 + 7\,755\,552R_2R_3S_4 - 8\,197\,056R_2^3S_4 + 22\,176T_6 - 17\,136R_2T_5.$$

$$\hat{F}_8/480 = 4\,163\,720\,988R_9 - 18\,578\,876\,400R_2R_8 - 13\,257\,132\,336R_3R_7 + 47\,044\,563\,552R_2^2R_7 - 11\,323\,099\,872R_4R_6 + 68\,987\,497\,824R_2R_3R_6 - 89\,763\,496\,704R_2^3R_6 - 5\,393\,204\,460R_5^2 + 60\,939\,180\,288R_2R_4R_5 + 26\,156\,846\,520R_3^2R_5 - 204\,571\,273\,536R_2^2R_3R_5 + 24\,254\,367\,984R_3R_4^2 - 94\,860\,853\,416R_2^2R_4^2 - 163\,159\,909\,920R_2R_3^2R_4 - 11\,694\,961\,908R_3^4 + 145\,249\,394\,472R_2^4R_5 + 464\,082\,286\,752R_2^3R_3R_4 + 199\,853\,845\,632R_2^2R_3^3 - 214\,309\,758\,096R_2^5R_4 - 462\,027\,698\,496R_2^4R_3^2 + 306\,582\,555\,888R_2^6R_3 - 58\,374\,657\,054R_2^8 + 121\,942\,296S_8 - 364\,275\,072R_2S_7 - 182\,025\,648R_3S_6 + 577\,403\,568R_2^2S_6 - 94\,328\,640R_4S_5 - 39\,671\,856R_5S_4 + 512\,942\,976R_2R_3S_5 + 199\,662\,624R_2R_4S_4 - 602\,775\,936R_2^3S_5 + 85\,580\,712R_3^2S_4 - 603\,997\,632R_2^2R_3S_4 + 390\,287\,520R_2^4S_4 + 1\,187\,928T_7 - 1\,800\,288R_2T_6 - 333\,648R_3T_5 + 933\,408R_2^2T_5 - 72\,324\,S_4^2 + 2\,268U_6.$$

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