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Abstract. Exact expressions are given for the free energy of the classical Heisenberg model in one lattice dimension and two or three spin dimensions with general anisotropy; the two-dimensional result, already known, is in terms of Mathieu functions and the three-dimensional result in terms of Lamé wavefunctions. The method presented solves the eigenvalue problem for an appropriate transfer matrix by relating it to solutions of the Helmholtz equation in suitable curvilinear coordinate systems. High and low temperature limits are discussed for the three-dimensional spin case and the connection given with already known results for partial anisotropy.

1. Introduction

The classical Heisenberg model consists of a one-dimensional lattice of N unit dipoles, each dipole being allowed to point in any direction in an n-dimensional vector space and each interacting with only its nearest neighbours. The hamiltonian for this classical system may be written

$$H_N = -\sum_{i=1}^{N} (J_1 x_1(i)x_1(i+1) + J_2 x_2(i)x_2(i+1) + \ldots + J_n x_n(i)x_n(i+1)) \quad (1)$$

where $x_j(i)$ indicates the jth direction component of the ith dipole and the J_j are interaction constants. The partition function and correlation functions for systems of this type have been investigated by several authors: for $n = 2$ by Joyce (1967a), for $n = 3$ and two of the J's taken equal by Joyce (1967a) and Thompson (1968) and for general values of n with all J's equal by Stanley (1969) and Stanley et al (1970).

For a line of N dipoles of which the Nth has components $x_1(N), \ldots, x_n(N)$ the partition function is

$Z_N(x_1(N), \ldots, x_n(N))$

$$= \int \frac{d\Omega_1}{\sigma} \ldots \int \frac{d\Omega_{N-1}}{\sigma} \exp v \sum_{i=1}^{N-1} (J_1 x_1(i)x_1(i+1) + \ldots + J_n x_n(i)x_n(i+1))$$

where $d\Omega_i$ is the surface element of the unit sphere for the ith dipole vector $(x_1(i), \ldots, x_n(i))$, σ the corresponding total surface area and $v = 1/kT$, T being the temperature. The

corresponding expression for $N+1$ dipoles is related to the above by

$$Z_{N+1}(x_1(N+1), \ldots, x_n(N+1))$$

$$= \int \frac{\mathrm{d}\Omega_N}{\sigma} \exp v(J_1 x_1(N)x_1(N+1) + \ldots + J_n x_n(N)x_n(N+1))$$

$$\times Z_N(x_1(N), \ldots, x_n(N))$$

so that the 'transfer matrix' for this system is the integral operator $\mathscr{J}$ given by

$$[\mathscr{J}_f](x_1, \ldots, x_n) = \int \frac{\mathrm{d}\Omega'}{\sigma} \exp v(J_1 x_1 x_1' + \ldots + J_n x_n x_n')f(x_1', \ldots, x_n') \qquad (2)$$

the integral being taken over the unit sphere. This operator is of Hilbert–Schmidt type so that its eigenvalues are real and, with the usual inner product, there is a complete orthonormal set of eigenvectors. Further, the kernel in (2) is positive so by Jentzsch's theorem (Jentzsch 1912) there is a simple positive maximum eigenvalue and this is an analytic function of v and $J_1, \ldots, J_n$. This analogue of the Perron–Frobenius theorem underlies the usual proofs that a one-dimensional system such as (1) cannot have a thermodynamic phase transition at finite temperatures (Münster 1969). A knowledge of the eigenvalues $\lambda_0, \lambda_1, \ldots$ of $\mathscr{J}$ and of the corresponding eigenvectors allows calculation of the partition function and correlation functions. In particular, the partition function for N dipoles with cyclic boundary conditions is given by

$$Z_N = \sum_{j=0}^{\infty} \lambda_j^N.$$

In the thermodynamic limit only the maximum eigenvalue λ_0 contributes and the free energy is given by

$$-vf(v, J_1, \ldots, J_n) = \lim_{N \to \infty} \frac{1}{N} \ln Z_N = \ln \lambda_0. \qquad (3)$$

It seems impossible to solve the eigenvalue problem for $\mathscr{J}$ in the general case but by establishing a connection with Helmholtz's equation we are able to present below the solutions for $n = 2$ and $n = 3$. In § 2 we illustrate the argument for the case $n = 2$ where the results are known in terms of Mathieu functions (Joyce 1967a) and § 3 carries through the same procedure for $n = 3$ where the appropriate functions are Lamé wavefunctions. Since the latter model includes some known special cases, various limiting forms and high and low temperature expansions are outlined in § 4. Finally, we summarize the results obtained and the difficulties in proceeding further. The main properties of Lamé wavefunctions are collected together in an appendix.

2. The planar model ($n = 2$)

The eigenvalue equation for $\mathscr{J}$ in the case $n = 2$ may be written from (2) as

$$\int \frac{\mathrm{d}\Omega'}{2\pi} \exp v(J_1 xx' + J_2 yy')h(x', y') = \lambda h(x, y). \qquad (4)$$

We denote the kernel by $W = \exp v(J_1 xx' + J_2 yy')$ and without loss of generality assume $J_1^2 \geqslant J_2^2$. Putting $\xi = J_1 x$, $\eta = J_2 y$ we have

$$\frac{\partial^2 W}{\partial \xi^2} + \frac{\partial^2 W}{\partial \eta^2} = v^2 (x'^2 + y'^2) W = v^2 W. \tag{5}$$

As x, y vary over the unit circle $x^2 + y^2 = 1$ the variables ξ, η vary over an ellipse so it is reasonable to introduce elliptic coordinates (Abramowitz and Stegun 1965)

$$\xi = \rho \cosh u \cos v \qquad \eta = \rho \sinh u \sin v \tag{6}$$

corresponding to

$$\begin{aligned} x &= \cos v & J_1 &= \rho \cosh u \\ y &= \sin v & J_2 &= \rho \sinh u. \end{aligned} \tag{7}$$

We take $0 \leqslant v \leqslant 2\pi$ and allow ρ, u all real values to cover the possible values of J_1, J_2. In terms of these variables equation (5) becomes

$$\frac{\partial^2 W}{\partial u^2} + \frac{\partial^2 W}{\partial v^2} - \tfrac{1}{2}\rho^2 v^2 (\cosh 2u - \cos 2v) W = 0$$

and assuming solutions of the form $W = f(u)g(v)$ one obtains

$$\frac{d^2 f}{du^2} - (a + \tfrac{1}{2}v^2 \rho^2 \cosh 2u) f = 0 \tag{8}$$

$$\frac{d^2 g}{dv^2} + (a + \tfrac{1}{2}v^2 \rho^2 \cos 2v) g = 0 \tag{9}$$

where a is a separation constant. Equation (9) is Mathieu's equation and (8) Mathieu's modified equation (we follow the notation of Abramowitz and Stegun 1965, chap 20). For the solution of (9) we want periodic functions and this determines the values of a as Sturm–Liouville eigenvalues. The solutions are

$$\begin{aligned} \mathrm{ce}_n(v, -\tfrac{1}{4}\rho^2 v^2) \qquad & n = 0, 1, 2, \ldots \\ \mathrm{se}_n(v, -\tfrac{1}{4}\rho^2 v^2) \qquad & n = 1, 2, \ldots \end{aligned}$$

with corresponding eigenvalues $a = a_n, a = b_n$ given in Abramowitz and Stegun (1965, § 20.2.26). Now (8) must be solved with these values of a. Corresponding to a_n, b_n the solutions are of type $\mathrm{Ce}_n(u)$, $\mathrm{Se}_n(u)$ respectively (we drop for the moment the second Mathieu parameter which here is always $-\tfrac{1}{4}\rho^2 v^2$). It follows that W may be expanded in the form

$$W = \sum_{r=0} \gamma_r \mathrm{Ce}_r(u)\mathrm{ce}_r(v) + \sum_{r=1} \delta_r \mathrm{Se}_r(u)\mathrm{se}_r(v).$$

Exactly the same procedure may be carried out in terms of x', y' in place of x, y but keeping the same J_1, J_2 and hence the same ρ, u. This gives an expansion of W of the form

$$W = \sum_{r=0}' \alpha_r \mathrm{Ce}_r(u)\mathrm{ce}_r(v)\mathrm{ce}_r(v') + \sum_{r=1} \beta_r \mathrm{Se}_r(u)\mathrm{se}_r(v)\mathrm{se}_r(v') \tag{10}$$

where α_r, β_r are now independent of u, v, v'. Now the functions $ce_r(v), se_r(v)$ form a complete orthogonal set for the interval $0 \leqslant v \leqslant 2\pi$ with orthogonality relations of the type

$$\int_0^{2\pi} ce_r(v)ce_s(v)\,dv = \pi\delta_{rs}. \tag{11}$$

From (4), (10) and (11) it follows that $ce_r(v)$, $r = 0, 1, \ldots$ and $se_r(v)$, $r = 1, 2, \ldots$ are a complete set of eigenfunctions for our operator $\mathscr{J}$ and that the corresponding eigenvalues are $\frac{1}{2}\alpha_r Ce_r(u)$ and $\frac{1}{2}\beta_r Se_r(u)$ respectively. There remains only to find explicit values for α_r, β_r and this is done most easily by choosing special values of the variables in (10). For example, by putting $u = 0$, $v' = \frac{1}{2}\pi$, multiplying by $ce_{2s}(v)$ and integrating, we obtain

$$\int_0^{2\pi} ce_{2s}(v)\,dv = \pi\alpha_{2s}Ce_{2s}(0)ce_{2s}(\tfrac{1}{2}\pi).$$

From the general properties of Mathieu functions (Abramowitz and Stegun 1965) this gives our eigenvalue in the form

$$\tfrac{1}{2}\alpha_{2s}Ce_{2s}(u) = \frac{1}{2\pi}\frac{2\pi A_0^{2s}}{ce_{2s}(0)ce_{2s}(\tfrac{1}{2}\pi)}Ce_{2s}(u) = (-1)^s Mc_{2s}^{(1)}(u) \tag{12}$$

where $Mc^{(1)}$ is a tabulated modified Mathieu function. In a similar way the other eigenvalues can be found and the complete list is $(i)^r Mc_r^{(1)}(u)$, $r = 0, 1 \ldots$ and $(i)^r Ms_r^{(1)}(u)$, $r = 1, 2, \ldots$.

Since by Jentzsch's theorem the maximum eigenvalue must remain non-degenerate even for $v \to 0$ it is clear that this eigenvalue is $Mc_0^{(1)}(u, -\frac{1}{4}\rho^2 v^2)$. These results have already been obtained by Joyce (1967a) who outlined some of their consequences so we will discuss them no further in this article.

3. The free energy of the Heisenberg model ($n = 3$)

When the dipoles are allowed to orientate themselves in a three-dimensional space ($n = 3$) the 'transfer matrix' $\mathscr{J}$ of (2) has an eigenvalue equation of the form

$$\int \frac{d\Omega'}{4\pi} \exp[v(axx'+byy'+czz')]h(x', y', z') = \lambda h(x, y, z) \tag{13}$$

the integral now being over the surface of the unit sphere. In this case we write the kernel $W = \exp v(axx'+byy'+czz')$ and assume, without restriction, that $a^2 \geqslant b^2 \geqslant c^2$. If we now put $\xi = ax$, $\eta = by$, $\zeta = cz$ we again arrive at the Helmholtz equation

$$\frac{\partial^2 W}{\partial\xi^2}+\frac{\partial^2 W}{\partial\eta^2}+\frac{\partial^2 W}{\partial\zeta^2} = v^2(x'^2+y'^2+z'^2)W = v^2 W. \tag{14}$$

As x, y, z vary over the surface of the unit sphere ξ, η, ζ vary over the surface of an ellipsoid, so it is reasonable to introduce confocal ellipsoidal coordinates α, β, γ related to ξ, η, ζ

by (in the notation of Erdelyi *et al* 1955)

$$\xi = k^2(a^2-c^2)^{1/2}\mathrm{sn}\alpha\,\mathrm{sn}\beta\,\mathrm{sn}\gamma$$

$$\eta = -\frac{k^2}{k'}(a^2-c^2)^{1/2}\mathrm{cn}\alpha\,\mathrm{cn}\beta\,\mathrm{cn}\gamma \tag{15}$$

$$\zeta = \frac{\mathrm{i}}{k'}(a^2-c^2)^{1/2}\mathrm{dn}\alpha\,\mathrm{dn}\beta\,\mathrm{dn}\gamma.$$

Here $k^2 = (a^2-b^2)/(a^2-c^2)$, $k'^2 = (b^2-c^2)/(a^2-c^2)$, $0 \leqslant k \leqslant 1$ and the jacobian elliptic functions are all of modulus k. If α varies between $\mathrm{i}K'$ and $K+\mathrm{i}K'$, β between K and $K+2\mathrm{i}K'$ and γ from 0 to $4K$ there is a one-to-one correspondence between the curvilinear coordinates α, β, γ and the cartesian ξ, η, ζ (K and K' are the usual complete elliptic integrals).

In terms of these coordinates the equation (14) becomes

$$\sum_{\alpha,\beta,\gamma\,\mathrm{cyclic}} (\mathrm{sn}^2\beta - \mathrm{sn}^2\gamma)\frac{\partial^2 W}{\partial\alpha^2} = -v^2k^4(a^2-c^2)(\mathrm{sn}^2\alpha-\mathrm{sn}^2\beta)(\mathrm{sn}^2\beta-\mathrm{sn}^2\gamma)(\mathrm{sn}^2\gamma-\mathrm{sn}^2\alpha)W.$$

Assuming a solution of the form $A(\alpha)B(\beta)C(\gamma)$ we have

$$\frac{\mathrm{d}^2 A}{\mathrm{d}\alpha^2} - (s + rk^2\mathrm{sn}^2\alpha + l^2v^2k^4\mathrm{sn}^4\alpha)A = 0 \tag{16}$$

and two other equations of this kind for $B(\beta)$ and $C(\gamma)$ all involving the same separation constants s, r and having $l^2 = a^2 - c^2$. The solutions of interest here (see Erdelyi *et al* 1955, § 15.1.1.) are doubly periodic and this determines the allowed values of s and r. The solutions themselves are ellipsoidal wavefunctions: these functions have been little studied but we collect some relevant known results in an appendix which the reader should consult for notation and references. From (16) it is reasonable to look for an expansion of the kernel in the form

$$W = \sum_{t,n,m} a_{t,n,m}\mathrm{el}_n^m(\alpha)\mathrm{el}_n^m(\beta)\mathrm{el}_n^m(\gamma)$$

where in each term the three ellipsoidal wavefunctions in the product are precisely the same, and where the summation is over all eight types of function (say $t = 1, \ldots, 8$) and over $n = 0, 1, 2, \ldots$ and the appropriate range of m for each n. Now this expansion is in terms of variables (15) which we may rewrite as

$$x = k\,\mathrm{sn}\beta\,\mathrm{sn}\gamma \qquad a = kl\,\mathrm{sn}\alpha$$

$$y = \mathrm{i}\frac{k}{k'}\mathrm{cn}\beta\,\mathrm{cn}\gamma \qquad b = \mathrm{i}kl\,\mathrm{cn}\alpha \tag{17}$$

$$z = \frac{1}{k'}\mathrm{dn}\beta\,\mathrm{dn}\gamma \qquad c = \mathrm{i}l\,\mathrm{dn}\alpha$$

(α now takes any value appropriate to the magnitude and sign of a, b, c) but we could just as well have expanded in terms of primed variables $\xi' = ax'$, $x' = k\,\mathrm{sn}\beta'\,\mathrm{sn}\gamma'$, etc. In this way, just as in (10), we obtain

$$W = \sum_{t,n,m} b_{t,n,m}\mathrm{el}_n^m(\alpha)\mathrm{elp}_n^m(\beta,\gamma)\mathrm{elp}_n^m(\beta',\gamma') \tag{18}$$

where each term is now a product of five identical ellipsoidal wavefunctions and the sum is over all eight types and all indices appropriate to each type. The coefficients b, which are independent of α, β, β', γ, γ', are more difficult to evaluate than in the case of Mathieu functions.

In going over to coordinates (17) the spherical surface element $d\Omega'$ becomes $ik^2(\mathrm{sn}^2\gamma'-\mathrm{sn}^2\beta')\,d\beta'\,d\gamma'$ so in view of the orthogonality properties of $\mathrm{elp}(\beta,\gamma)$ (see appendix (A.3)) it is now apparent that the eigenfunctions of $\mathscr{J}$ expressed in the new coordinates are simply all the ellipsoidal surface wavefunctions $\mathrm{elp}_n^m(\beta,\gamma)$ and the corresponding eigenvalues, obtained from the appropriate term of (18), are

$$-\frac{k^2\epsilon}{8\pi}b_{t,n,m}\,\mathrm{el}_n^m(\alpha). \tag{19}$$

By Jentzsch's theorem the maximum eigenvalue must remain non-degenerate in the limit $v\to 0$ in which the functions $\mathrm{elp}(\beta,\gamma)$ go over to products of Lamé polynomials; the properties of the latter show that the eigenfunction with maximum eigenvalue is, in full notation, $\mathrm{uelp}_0^0(\beta,\gamma)$. To obtain the corresponding eigenvalue we need to know the appropriate coefficient b in series (18) and, as in § 2, this can be done by choosing special values for the variables. We put $\alpha = K+iK'$, $\beta = K$, $\gamma = 0$ so all terms in (18) vanish except those involving only the functions uel_{2n}^m. Thus

$$1 = \sum_{n=0}^{\infty}\sum_{m=0}^{n} b_{1,2n,m}\mathrm{uel}_{2n}^m(K+iK')\mathrm{uelp}_{2n}^m(K,0)\mathrm{uelp}_{2n}^m(\beta',\gamma').$$

If this is multiplied by $(\mathrm{sn}^2\gamma'-\mathrm{sn}^2\beta')\mathrm{uelp}_{2n}^m(\beta',\gamma')$ and integrated over S then by (A.3), (A.5) we obtain

$$-ib_{1,2n,m}\mathrm{uel}_{2n}^m(K+iK')\mathrm{uelp}_{2n}^m(K,0)$$

$$= \iint_S (\mathrm{sn}^2\gamma'-\mathrm{sn}^2\beta')\mathrm{elp}_{2n}^m(\beta',\gamma')\,d\beta'\,d\gamma' = -iA_0^0\left(\frac{8\pi}{k^2}\right)^{1/2}$$

where A_0^0 is the first coefficient in the expansion of uelp_{2n}^m in a series of type (A.4). In particular, the maximum eigenvalue λ_0 is given by $n = m = 0$

$$\lambda_0 = \left(\frac{k^2}{8\pi}\right)^{1/2}\frac{A}{\mathrm{uel}_0^0(K+iK')\mathrm{uelp}_0^0(K,0)}\mathrm{uel}_0^0(\alpha) \tag{20}$$

where A is now the first coefficient in the expansion of uelp_0^0. The result (20) is to be compared with (12) and leads to an exact expression for the free energy (3) of the Heisenberg model for $n = 3$.

4. High and low temperature series and limiting cases

The exact solution obtained in the preceding section involves ellipsoidal wavefunctions about which not a great deal is known. Some explicit information is available however for large and small values of v which correspond to low and high temperatures respectively. Further, if two of the interaction parameters a, b, c are put equal in (13) the expressions in § 3 ought to reduce to known results in terms of simpler functions. We now discuss these topics in turn.

A series expansion of uel_0^0 appropriate for small values of v is given in (A.6) and this may be inserted directly for the ellipsoidal wavefunctions in (20). By inserting (A.6) into (A.5) a suitable series is also obtained for the constant A occurring in (20). A considerable amount of tedious but elementary algebra is needed in simplifying the result and we merely quote the final answer:

$$\lambda_0 = 1 + e_1 l^2 v^2 + e_2 l^4 v^4 + e_3 l^6 v^6 + \mathrm{O}(v^8) \tag{21}$$

where

$$e_1 = \frac{k^2 \mathrm{sn}^2\alpha}{6} - \frac{(1+k^2)}{18}$$

$$e_2 = \frac{k^4 \mathrm{sn}^4\alpha}{120} - \frac{k^2(1+k^2)\mathrm{sn}^2\alpha}{180} + \frac{67k^4 - 22k^2 + 67}{16200}$$

$$e_3 = \frac{k^6 \mathrm{sn}^6\alpha}{5040} - \frac{k^4(1+k^2)\mathrm{sn}^4\alpha}{5040} + \frac{(83k^4 - 38k^2 + 83)k^2\mathrm{sn}^2\alpha}{226\,800}$$

$$- \frac{(3037k^4 - 2038k^2 + 3037)(1+k^2)}{14\,288\,400}.$$

The low temperature case is not so easily disposed of as the existing asymptotic series of $\mathrm{el}(z)$ for large v all break down at certain transition points such as $z = K$ in the complex plane. The dominant term, however, can be obtained by using only the leading term in the asymptotic expansion of $\mathrm{uel}_0^0(z)$ which for z in the ranges 0 to K and K to $K + \mathrm{i}K'$ is given by (Arscott and Sleeman 1970)

$$\mathrm{uel}_0^0(z) \sim \text{constant} \times \exp(vlk\,\mathrm{sn}z)(1 + k\,\mathrm{sn}z)^{-1/2}(1 + \mathrm{sn}z)^{-1/2}.$$

This form is substituted into the eigenvalue equation (13) which according to § 3 can be written

$$\iint\limits_S \exp\left(\frac{vl}{k'^2}(k^3 k'^2 \mathrm{sn}\alpha\,\mathrm{sn}\beta\,\mathrm{sn}\gamma\,\mathrm{sn}\beta'\,\mathrm{sn}\gamma' - \mathrm{i}k^3 \mathrm{cn}\alpha\,\mathrm{cn}\beta\,\mathrm{cn}\gamma\,\mathrm{cn}\beta'\,\mathrm{cn}\gamma' + \mathrm{i}\,\mathrm{dn}\alpha\,\mathrm{dn}\beta\,\mathrm{dn}\gamma\,\mathrm{dn}\beta'\,\mathrm{dn}\gamma')\right)$$

$$\times (\mathrm{sn}^2\gamma' - \mathrm{sn}^2\beta')\mathrm{uelp}_0^0(\beta', \gamma')\,\mathrm{d}\beta'\,\mathrm{d}\gamma' = -\frac{8\pi\mathrm{i}}{k^2}\lambda_0\mathrm{uelp}_0^0(\beta, \gamma).$$

With $\gamma = K$, $\beta = K + \mathrm{i}K'$ this simplifies to

$$\iint\limits_S \exp[vk^2 l\,\mathrm{sn}\alpha\,\mathrm{sn}\beta'\,\mathrm{sn}\gamma'](\mathrm{sn}^2\gamma' - \mathrm{sn}^2\beta')\mathrm{uelp}_0^0(\beta', \gamma')\,\mathrm{d}\beta'\,\mathrm{d}\gamma'$$

$$= -\frac{8\pi\mathrm{i}}{k^2}\lambda_0\mathrm{uelp}_0^0(K + \mathrm{i}K', K). \tag{22}$$

The leading term of the left-hand side for large v is easily evaluated by the method of steepest descent and is found to be

$$\frac{-4\pi\mathrm{i}\exp(|vlk\,\mathrm{sn}\alpha|)}{vlk^2(1 + k\,\mathrm{sn}\alpha)^{1/2}(k + k\,\mathrm{sn}\alpha)^{1/2}}\mathrm{uelp}_0^0(K + \mathrm{i}K', K). \tag{23}$$

Expression (23) in conjunction with equation (22) provides the dominant behaviour of the maximum eigenvalue for large v

$$\lambda_0 \simeq \frac{\exp(vlk|\text{sn}\alpha|)}{2vl(1+k\text{sn}\alpha)^{1/2}(k+k\text{sn}\alpha)^{1/2}}\left(1+\text{O}\left(\frac{1}{v}\right)\right). \tag{24}$$

This leads to an energy per dipole

$$E \simeq -kl|\text{sn}\alpha| + \frac{1}{v} + \text{O}\left(\frac{1}{v^2}\right) = -\max(|a|,|b|,|c|) + \frac{1}{v} + \text{O}\left(\frac{1}{v^2}\right).$$

The energy at $T = 0$ is just what is expected for a hamiltonian of the form (1). If a is positive and of greatest magnitude, there are two zero temperature dipole states, with all dipoles pointing in the $+x$ or all in the $-x$ directions; if a is negative the two antiferromagnetic ground states have the dipoles pointing alternately in the $+x$ and $-x$ directions.

Next we examine the possibility of having two of the interaction strengths equal. From (17) it appears that the case $a = b$ requires $k = 0$ while $b = c$ requires $k = 1$; we carry through the details only for the first of these, the oblate case, and for simplicity assume a, b, c all positive so that α may be taken to vary in the range iK' to $iK'+K$. As $k \to 0$, $K \to \frac{1}{2}\pi$ while $K' \to \infty$; we therefore change variables from α to $v = \alpha - iK'$ and take the limit $k \to 0$ holding v fixed. A simple calculation gives

$$a = kl\,\text{sn}\alpha \to l\,\text{cosec}\,v$$

$$b = ikl\,\text{cn}\alpha \to l\,\text{cosec}\,v \qquad 0 \leqslant v \leqslant \frac{1}{2}\pi.$$

$$c = il\,\text{dn}\alpha \to l\,\text{cot}\,v$$

We may now compare this with the approach of Joyce (1967a) and find that the two notations are related by $J_\perp = l/(2\sin v)$ and $\tanh\rho = \cos v$. From our appendix we have that the function $\text{uel}_0^0(\beta, v^2l^2)$ occurring in the maximum eigenfunction reduces as $k \to 0$ to $\text{Ps}_0^0(x, -v^2l^2)$ and this is in accord with Joyce's $S_{00}(2J_\perp/kT\cosh\rho, x)$; the other functions go over to spheroidal wavefunctions in a similar fashion. Further, one may check quite easily that for $k = 0$ the high temperature series (21) becomes that given by Joyce (1967b) and the low temperature result (24) agrees, as far as it goes, with the expressions given by Joyce (1967a) and Thompson (1968).

5. Conclusions

In the preceding sections we have obtained, in terms of ellipsoidal wavefunctions, exact expressions for the eigenvectors and eigenvalues of a transfer matrix for the general $n = 3$ classical Heisenberg model and hence an expression for the free energy of this system. Although not much is known about these functions some explicit information can be extracted in the high and low temperature limits and this was given in § 4. It is interesting that such complicated functions arise in an apparently simple problem; these ellipsoidal wavefunctions are about the most complicated special functions that have been studied and this fact suggests that the method used in this article will be impracticable for more complicated models. For $n > 3$ appropriate functions have not yet been studied and the method will work only in the special case where all the interaction constants are equal, when it will reproduce the results of Stanley (1969) for general n.

No exact results have ever been obtained for a classical Heisenberg model with a magnetic field except in the Ising case $n = 1$. If the present method is followed in, for example, the isotropic $n = 2$ case one is led very naturally to consider the bipolar coordinate system. It is perhaps significant that the Helmholtz equation is not separable in these coordinates and the method will not carry through.

It appears then that although the method presented in this article disposes of the $n = 2$ and $n = 3$ cases it does not offer much hope for a solution of more complicated Heisenberg models. It may however be applicable to other types of models. Finally we may remark that in finding the free energy we have not fully exploited the information available from the eigenvectors and eigenvalues in the case $n = 3$; we may for example hope to obtain some properties of correlation functions. Although the analysis involved in this has proved rather complicated we hope to present it in a future publication.

Appendix. Ellipsoidal wavefunctions

Ellipsoidal or Lamé wavefunctions are the uniform doubly-periodic solutions of the differential equation (16) which we now write in the notation

$$\frac{d^2 W}{dz^2} - (a + bk^2\text{sn}^2z + qk^4\text{sn}^4z)W = 0. \tag{A.1}$$

After the initial study of these functions by Möglich (1927) and Malurkar (1935) little more appears to have been done until Arscott (1964) revived the subject about 1955. Here we follow Arscott's notation and classification scheme. The ellipsoidal wavefunctions are all of the form

$$\text{el}(z) = \text{sn}^\lambda(z)\text{cn}^\mu(z)\text{dn}^\nu(z)F(\text{sn}^2z) \tag{A.2}$$

where λ, μ, ν may be either 0 or 1 and F is an integral function of its argument. Accordingly, they can be classified under eight types by their parity at $z = 0$ and their periods. The symbols $\text{el}(z)$ or $\text{el}_n^m(z)$ denote any ellipsoidal wavefunction and the eight types are prefixed by one or more of the letters u, s, c, d as shown in table 1. With the indices labelled as below n runs over the non-negative integers and m takes, in all cases, the values 0, 1, ..., n.

Table 1. Types of ellipsoidal wavefunctions.

Type	Parity	Periods	Type	Parity	Periods
uel_{2n}^m	even	$2K, 2iK'$	scel_{2n+2}^m	odd	$2K, 4iK'$
sel_{2n+1}^m	odd	$4K, 2iK'$	sdel_{2n+2}^m	odd	$4K, 4iK'$
cel_{2n+1}^m	even	$4K, 4iK'$	cdel_{2n+2}^m	even	$4K, 2iK'$
del_{2n+1}^m	even	$2K, 4iK'$	scdel_{2n+3}^m	odd	$2K, 2iK'$

These functions exist for all real values of q and suitable q-dependent values of a, b and are in one-to-one correspondence with the Lamé polynomials to which they reduce when $q = 0$. A product $\mathrm{el}(\beta)\mathrm{el}(\gamma)$ where el denotes precisely the same function is abbreviated to $\mathrm{elp}(\beta, \gamma)$ with, if necessary, prefix and indices as above. Functions elp of different types or with different indices are orthogonal and are normalized so that when the left-hand side is nonzero we have

$$\iint_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)(\mathrm{elp}(\beta, \gamma))^2 \, \mathrm{d}\beta \, \mathrm{d}\gamma = \mathrm{i}\epsilon \tag{A.3}$$

where S denotes the field of integration γ from $-2K$ to $2K$, β from $K - 2\mathrm{i}K'$ to $K + 2\mathrm{i}K'$ and ϵ is ± 1 accordingly as cn z is or is not a factor of $\mathrm{el}(z)$ (thus $\epsilon = (-1)^{\mu+1}$, μ as in A.2).

Many of the properties of ellipsoidal wavefunctions have been obtained by the use of certain integral equations. In this way Möglich (1927) found expansions of elp in terms of spherical surface harmonics and of el in Legendre functions of argument dn$z$ and also in spherical Bessel functions; similarly Arscott (1959) derived an expansion in terms of Lamé polynomials and this is the only one we will write out here. If we denote Lamé polynomials by the general symbol $\mathrm{E}(z)$ and adorn this in a manner consistent with that used above for $\mathrm{el}(z)$ (thus $\lim_{q \to 0} \mathrm{uel}_{2n}^m(z) = \mathrm{uE}_{2n}^m(z)$, etc) the expansion for $\mathrm{uelp}_{2N}^M(\beta, \gamma)$ is written

$$\mathrm{uelp}_{2N}^M(\beta, \gamma) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} A_n^m \mathrm{uEp}_{2n}^m(\beta, \gamma) \tag{A.4}$$

and similarly in the other cases. The coefficients A, dependent on N, M, q and the type, are determined by a three-term recurrence relation in which the terms are matrices, which renders this vastly more complicated than the Mathieu case. On multiplying (A.4) by $(\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)\mathrm{uEp}_0^0(\beta, \gamma)$ and integrating over S orthonormality of Ep (Arscott 1959) gives the useful result

$$\iint_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)\mathrm{uelp}_{2N}^M(\beta, \gamma) \, \mathrm{d}\beta \, \mathrm{d}\gamma = -\mathrm{i}A_0^0 \left(\frac{8\pi}{k^2}\right)^{1/2}. \tag{A.5}$$

By working directly with the differential equation (A.1) both Malurkar and Arscott have obtained series expansions of $\mathrm{el}(z)$ for small values of q (Malurkar 1935, Arscott 1956) and asymptotic expansions for large q (Malurkar 1935, Arscott and Sleeman 1970). The low q expansion for uel_0^0, adjusted to present normalization, may be written

$$\frac{\mathrm{uel}_0^0(z)}{\mathrm{uel}_0^0(0)} = 1 + q\frac{k^2\mathrm{sn}^2z}{6} + q^2\left(\frac{k^4\mathrm{sn}^4z}{120} + \frac{k^2(1+k^2)\mathrm{sn}^2z}{270}\right)$$
$$+ q^3\left(\frac{k^6\mathrm{sn}^6z}{2^4 \cdot 3^2 \cdot 5 \cdot 7} + \frac{k^4(1+k^2)\mathrm{sn}^4z}{2^2 \cdot 3^3 \cdot 5 \cdot 7} - \frac{k^2(1-4k^2+k^4)\mathrm{sn}^2z}{3^5 \cdot 5 \cdot 7}\right) + O(q^4). \tag{A.6}$$

This series converges for small q but the radius of convergence is not known. The high q expansions given in the literature contain a number of errors and in any case provide series which are not valid in the neighbourhood of points such as $z = 0$ needed in (20); they are not used in this article.

Finally we mention that in the limits $k \to 0$ and $k \to 1$ the ellipsoidal wavefunctions go over to spheroidal wavefunctions (Möglich 1927, Sleeman 1967). We illustrate this connection for $\mathrm{uel}_{2n}^m(\beta; q, k^2)$ with $q > 0$ and β as in § 3. As $k \to 0$, $K' \to \infty$ so we change

to an appropriate real variable η given by $i\eta = \beta - K - iK'$; η then varies from $-K'$ to K'. By using properties of elliptic functions it is easy to see

$$\lim_{k \to 0} k \, \mathrm{sn}(\beta, k) = \lim_{k \to 0} \mathrm{dn}(\eta, k') = \mathrm{sech} \, \eta$$

so that for $k = 0$ equation (A.1) has become

$$\frac{\mathrm{d}^2 W}{\mathrm{d}\eta^2} + [(a+b+q) - (b+2q)\tanh^2\eta + q\tanh^4\eta] \, W = 0.$$

The further change of variable $x = \tanh \eta$ reveals this to be the spheroidal wave equation (Arscott 1964). The function $\mathrm{uel}_{2n}^m(\beta)$ has $2(n-m)$ zeros in $]K, K+2iK'[$ so its limit must have $2(n-m)$ zeros in $-1 < x < 1$. This shows that as $k \to 0$ $\mathrm{uel}_{2n}^m(\beta; q, k^2)$ goes over to the oblate angular spheroidal wavefunction $\mathrm{Ps}_{2n}^{2m}(x, -q)$ with appropriate normalization. Since the functions uel have the general property $\mathrm{uel}_{2n}^m(\eta; -q, k'^2) = \mathrm{uel}_{2n}^{n-m}(\beta; q, k^2)$ the above result also implies that as $k \to 1$, $\mathrm{uel}_{2n}^m(\beta; q, k^2)$ reduces to the prolate angular function $\mathrm{Ps}_{2n}^{2(n-m)}(x, q)$. In a similar way $\mathrm{uel}(\alpha)$, $\mathrm{uel}(\gamma)$ reduce to radial wavefunctions and trigonometric functions respectively.

References

Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)
Arscott F M 1956 *Q. J. Math., Oxford* **7** 161–74
—— 1959 *Proc. London Math. Soc.* **9** 21–50
—— 1964 *Periodic Differential Equations* (Oxford: Pergamon)
Arscott F M and Sleeman B D 1970 *Mathematika* **17** 39–46
Erdelyi A, Magnus W, Oberhettinger F and Tricomi F G 1955 *Higher Transcendental Functions* vol 3 (New York: McGraw-Hill)
Jentzsch R 1912 *Crelles J.* **141** 235–44
Joyce G S 1967a *Phys. Rev. Lett.* **19** 581–3
—— 1967b *Phys. Rev.* **155** 478–91
Malurkar S L 1935 *Indian J. Phys.* **9** 45–80, 251–4
Möglich F 1927 *Ann. Phys., Lpz* **83** 609–734
Münster A 1969 *Statistical Thermodynamics* vol 1 (Berlin: Springer-Verlag)
Sleeman B D 1967 *J. Inst. Maths Applics* **3** 4–15
Stanley H E 1969 *Phys. Rev.* **179** 570–7
Stanley H E, Blume M, Matsuno K and Milosevic S 1970 *J. Appl. Phys.* **41** 1278–80
Thompson C J 1968 *J. Math. Phys.* **9** 241–5