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Correlation functions of the classical Heisenberg model I. High temperature behaviour

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Abstract. The classical Heisenberg model, with one lattice and three spin dimensions, has recently been solved for general anisotropy in terms of ellipsoidal wavefunctions. These functions are used here to obtain exact expressions for the pair correlation functions and susceptibilities in the three spin directions. Explicit formulae, valid at high temperatures, are derived for these quantities on the basis of known series expansions for ellipsoidal functions and it is shown that these formulae reduce to known results in the partially anisotropic and isotropic cases.

1. Introduction

In a recent publication (Rae 1974) it was shown that the one-dimensional anisotropic classical Heisenberg model can be solved in terms of ellipsoidal wavefunctions by the transfer matrix technique. The Hamiltonian for the model may be taken as

$$H = -\sum_{j=1}^{N} (ax_jx_{j+1}+by_jy_{j+1}+cz_jz_{j+1}), \tag{1}$$

where (x_j, y_j, z_j) is a point on a unit sphere representing the orientation of the jth classical spin and a, b and c are interaction constants. The 'transfer matrix' for this model is an integral operator $\mathscr{I}$ given by

$$[\mathscr{I}f](x, y, z) = \int \frac{\mathrm{d}\Omega'}{4\pi} \exp[v(axx'+byy'+czz')]f(x', y', z'), \tag{2}$$

with $v = 1/k_{\mathrm{B}}T$, the inverse temperature, and the integral taken over the unit sphere. We parametrize the above Cartesian variables by ellipsoidal coordinates

$$\begin{aligned} x &= k \operatorname{sn}\beta \operatorname{sn}\gamma & a &= kl \operatorname{sn}\alpha \\ y &= \mathrm{i}\frac{k}{k_1} \operatorname{cn}\beta \operatorname{cn}\gamma & b &= \mathrm{i}kl \operatorname{cn}\alpha \\ z &= \frac{1}{k_1} \operatorname{dn}\beta \operatorname{dn}\gamma & c &= \mathrm{i}l \operatorname{dn}\alpha \end{aligned} \tag{3}$$

where β, γ now label the unit sphere and a, b, c are replaced by parameters k, l and α.

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The Jacobian elliptic functions are of modulus k with $k_1 = \sqrt{(1-k^2)}$. In terms of the new variables the eigenvalue equation for $\mathscr{I}$ is

$$\frac{\mathrm{i}k^2}{8\pi}\iint_S \exp\left(\frac{vl}{k_1^2}(k^3k_1^2 \operatorname{sn}\alpha \operatorname{sn}\beta \operatorname{sn}\gamma \operatorname{sn}\beta' \operatorname{sn}\gamma' - \mathrm{i}k^3 \operatorname{cn}\alpha \operatorname{cn}\beta \operatorname{cn}\gamma \operatorname{cn}\beta' \operatorname{cn}\gamma' + \mathrm{i} \operatorname{dn}\alpha \operatorname{dn}\beta \operatorname{dn}\gamma \operatorname{dn}\beta' \operatorname{dn}\gamma')\right)(\operatorname{sn}^2\gamma' - \operatorname{sn}^2\beta')f(\beta',\gamma')\,\mathrm{d}\beta'\,\mathrm{d}\gamma' = \lambda f(\beta,\gamma) \tag{4}$$

in which the field of integration S has γ' ranging from $-2K$ to $+2K$ and β' from $K-2\mathrm{i}K'$ to $K+2\mathrm{i}K'$, K and K' being the usual complete elliptic integrals. Equation (4) has as eigenfunction solutions the ellipsoidal surface wavefunctions elp(β, γ) of all eight types and with all allowed indices (for definitions and details see Arscott 1964 or Rae 1974). Knowledge of these eigenfunctions allows most properties of interest to be calculated for the model: this article examines some aspects of the pair correlation functions.

In the following section we define the pair correlation functions to be examined and obtain suitable expressions for them in terms of the eigenfunctions and eigenvalues mentioned above. Section 3 gives an account of the method of obtaining explicit high temperature series for the correlation function $\langle x_j x_{j+r}\rangle$ while § 4 gives the corresponding results for the y and z correlations and the x, y and z susceptibilities. In the concluding section we check the results by calculating $\langle H\rangle$ and show that the present results reduce to the known formulae in the extreme anisotropic and completely isotropic cases. The calculations in this article rely heavily on the evaluation of integrals of elliptic functions, the details of which are not given in the text. In an appendix we outline the technique used for these integrals and an example of its application.

2. The pair correlation functions

For convenience we suppose that the eigenvalues of equation (4), for a given value of v, are put in order of decreasing magnitude $\lambda_0, \lambda_1, \dots$ and that the corresponding eigenfunctions are labelled $f_0, f_1, \dots$ or, if we wish to indicate to which spin the argument belongs, $f_0(j)$ etc. The pair correlation function for x components is, if we choose cyclic boundary conditions,

$$\begin{aligned}\langle x_j x_{j+r}\rangle &= \lim_{N\to\infty}\frac{1}{Z_N}\int\frac{\mathrm{d}\Omega_1}{4\pi}\dots\int\frac{\mathrm{d}\Omega_N}{4\pi}x_j x_{j+r}\,\mathrm{e}^{-vH} \\ &= \lim_{N\to\infty}\frac{1}{Z_N}\int\frac{\mathrm{d}\Omega_1}{4\pi}\int\frac{\mathrm{d}\Omega_j}{4\pi}\int\frac{\mathrm{d}\Omega_{j+r}}{4\pi}W^{(j-1)}(1,j)x_j W^{(r)}(j,j+r)x_{j+r} \\ &\quad\times W^{(N+1-j-r)}(j+r,1)\end{aligned} \tag{5}$$

with Z_N the partition function and $W^{(r)}$ the rth iterated kernel, the kernel of $\mathscr{I}^r$. We may write with normalized eigenfunctions

$$W^{(r)}(k,l) = \sum_{n=0}^{\infty}\lambda_n^r f_n(k) f_n(l)$$

and for large N replace Z_N by λ_0^N so that

$$\langle x_j x_{j+r}\rangle = \lim_{N\to\infty} \frac{1}{Z_N} \sum_{n=0}^{\infty} \sum_{p=0}^{\infty} \lambda_n^{N-r} \lambda_p^r \left(\int \frac{d\Omega_j}{4\pi} f_p(j) x_j f_n(j) \right)^2$$
$$= \sum_{p=0}^{\infty} \left(\frac{\lambda_p}{\lambda_0} \right)^r \left(\int \frac{d\Omega_j}{4\pi} f_p(j) x_j f_0(j) \right)^2. \tag{6}$$

This last expression is, of course, independent of j.

In a similar way the correlation functions $\langle y_j y_{j+r}\rangle$ and $\langle z_j z_{j+r}\rangle$ have the same form as (6) but with the x_j inside the integral replaced by y_j and z_j respectively.

The integral $\int (d\Omega/4\pi) f_p x f_0$ will not always be nonzero. We know from previous work (Rae 1974) that f_0 corresponding to the maximum eigenvalue is the function $\mathrm{uelp}_0^0(\beta, \gamma)$ and from (3) we have $x = k \,\mathrm{sn}\, \beta \,\mathrm{sn}\, \gamma$. It follows that $x f_0$ has the same parities as the functions selp and by the completeness of ellipsoidal wavefunctions may be expanded in a series of selp functions. By orthogonality the only choices of f_p giving a nonzero result in (6) will be

$$\mathrm{selp}_{2n+1}^m(\beta, \gamma),$$

and as p runs over the values 0 to ∞, n and m run over the allowed values $n: 0 \ldots \infty$, $m: 0 \ldots n$. If we denote the corresponding eigenvalues by $\mathrm{s}\lambda_{2n+1}^m$ we may rewrite (6) as

$$\langle x_j x_{j+r}\rangle = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \left(\frac{\mathrm{s}\lambda_{2n+1}^m}{\lambda_0} \right)^r [I_{2n+1}^m]^2 \tag{7}$$

$$I_{2n+1}^m = \frac{\mathrm{i}k^2}{8\pi} \iint_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta) k \,\mathrm{sn}\, \beta \,\mathrm{sn}\, \gamma \,\mathrm{selp}_{2n+1}^m(\beta, \gamma) \,\mathrm{uelp}_0^0(\beta, \gamma) \,d\beta \,d\gamma. \tag{8}$$

An analogous argument gives for the y correlations, in an obvious notation,

$$\langle y_j y_{j+r}\rangle = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \left(\frac{\mathrm{c}\lambda_{2n+1}^m}{\lambda_0} \right)^r [J_{2n+1}^m]^2 \tag{9}$$

$$J_{2n+1}^m = \frac{\mathrm{i}k^2}{8\pi} \iint_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta) \frac{\mathrm{i}k}{k_1} \mathrm{cn}\, \beta \,\mathrm{cn}\, \gamma \,\mathrm{celp}_{2n+1}^m(\beta, \gamma) \,\mathrm{uelp}_0^0(\beta, \gamma) \,d\beta \,d\gamma, \tag{10}$$

and for the z correlations

$$\langle z_j z_{j+r}\rangle = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \left(\frac{\mathrm{d}\lambda_{2n+1}^m}{\lambda_0} \right)^r [K_{2n+1}^m]^2 \tag{11}$$

$$K_{2n+1}^m = \frac{\mathrm{i}k^2}{8\pi} \iint_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta) \frac{1}{k_1} \mathrm{dn}\, \beta \,\mathrm{dn}\, \gamma \,\mathrm{delp}_{2n+1}^m(\beta, \gamma) \,\mathrm{uelp}_0^0(\beta, \gamma) \,d\beta \,d\gamma. \tag{12}$$

For later use we also record here expressions for the self-correlation functions ($r = 0$). We have

$$\langle x_j^2\rangle = \lim_{N\to\infty} \frac{1}{Z_N} \int \frac{d\Omega_j}{4\pi} x_j^2 W^{(N)}(j,j) = \lim_{N\to\infty} \frac{1}{Z_N} \int \frac{d\Omega_j}{4\pi} x_j^2 \sum_{n=0}^{\infty} \lambda_n^N [f_n(j)]^2 = \int \frac{d\Omega_j}{4\pi} x_j^2 [f_0(j)]^2$$
$$= \frac{\mathrm{i}k^2}{8\pi} \iint_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta) k^2 \,\mathrm{sn}^2\beta \,\mathrm{sn}^2\gamma [\mathrm{uelp}_0^0(\beta, \gamma)]^2 \,d\beta \,d\gamma, \tag{13}$$

and similarly

$$\langle y_j^2\rangle = \frac{ik^2}{8\pi}\iint\limits_S (\mathrm{sn}^2\gamma-\mathrm{sn}^2\beta)\frac{(-1)k^2}{k_1^2}\mathrm{cn}^2\beta\,\mathrm{cn}^2\gamma[\mathrm{uelp}_0^0(\beta,\gamma)]^2\,\mathrm{d}\beta\,\mathrm{d}\gamma \tag{14}$$

$$\langle z_j^2\rangle = \frac{ik^2}{8\pi}\iint\limits_S (\mathrm{sn}^2\gamma-\mathrm{sn}^2\beta)\frac{1}{k_1^2}\mathrm{dn}^2\beta\,\mathrm{dn}^2\gamma[\mathrm{uelp}_0^0(\beta,\gamma)]^2\,\mathrm{d}\beta\,\mathrm{d}\gamma. \tag{15}$$

Alternative expressions may be obtained by setting $r = 0$ in (7), (9) and (11); these are related to (13), (14) and (15) by Parseval's theorem.

3. $\langle x_j x_{j+r}\rangle$ at high temperatures

The exact expressions (7), (8) are of little use unless more explicit forms are available for the eigenvalues and the integrals. For high temperatures such forms may be obtained from the standard expansions of el functions as power series in v. In order to calculate the correlation function we have to know: (i) which of $\mathrm{s}\lambda_{2n+1}^m$ is greatest for v small, (ii) an expansion for this $\mathrm{s}\lambda$; and (iii) expansions for the related integrals.

For point (i) above we may argue as follows. We let

$$f = g_0+vg_1+\ldots, \qquad \lambda = \mu_0+v\mu_1+\ldots$$

in the eigenvalue equation (4) and equate coefficients of equal powers of v. This yields

$$\frac{ik^2}{8\pi}\iint\limits_S (\mathrm{sn}^2\gamma'-\mathrm{sn}^2\beta')g_0(\beta',\gamma')\,\mathrm{d}\beta'\,\mathrm{d}\gamma' = \mu_0 g_0(\beta,\gamma), \tag{16}$$

$$\frac{ik^2}{8\pi}\iint\limits_S (\mathrm{sn}^2\gamma'-\mathrm{sn}^2\beta')(k^3 l\,\mathrm{sn}\,\alpha\,\mathrm{sn}\,\beta\,\mathrm{sn}\,\gamma\,\mathrm{sn}\,\beta'\,\mathrm{sn}\,\gamma'+\ldots)g_0\,\mathrm{d}\beta'\,\mathrm{d}\gamma'$$
$$+\frac{ik^2}{8\pi}\iint\limits_S (\mathrm{sn}^2\gamma'-\mathrm{sn}^2\beta')g_1\,\mathrm{d}\beta'\,\mathrm{d}\gamma' = \mu_1 g_0(\beta,\gamma)+\mu_0 g_1(\beta,\gamma) \tag{17}$$

and so on. It follows from (16) that unless g_0 is a constant μ_0 is zero. But the only elp function whose leading term is a constant is uelp_0^0 (Arscott 1956) so this is the eigenfunction corresponding to the maximum eigenvalue; this was already used in the calculation of the partition function (Rae 1974). With $\mu_0 = 0$ the equation (17) gives that either $\mu_1 = 0$ or $g_0(\beta,\gamma)$ is of the form

$$c_0+c_1\,\mathrm{sn}\,\beta\,\mathrm{sn}\,\gamma+c_2\,\mathrm{cn}\,\beta\,\mathrm{cn}\,\gamma+c_3\,\mathrm{dn}\,\beta\,\mathrm{dn}\,\gamma.$$

The series expansions for el functions (Arscott 1956) show that the only possibilities are $\mathrm{selp}_1^0, \mathrm{celp}_1^0, \mathrm{delp}_1^0$. We may continue the argument in this way to show that an eigenvalue corresponding to elp_n^m has a leading term of order v^n. Thus for the point (i) under consideration we need only $\mathrm{s}\lambda_1^0$ corresponding to $n = m = 0$.

From Arscott (1956) we have

$$N_0\,\mathrm{uel}_0^0(z) = 1+\tfrac{1}{6}v^2l^2k^2\,\mathrm{sn}^2 z+\mathrm{O}(v^4), \tag{18}$$

$$N_1\,\mathrm{sel}_1^0(z) = \mathrm{sn}\,z+\tfrac{1}{10}v^2l^2k^2\,\mathrm{sn}^3 z+\mathrm{O}(v^4), \tag{19}$$

where N_0 and N_1 are normalization constants to be determined by the normalization condition

$$\frac{ik^2}{8\pi}\iint_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)[\mathrm{elp}(\beta,\gamma)]^2 = 1.$$

A short calculation with (18) and (19) gives

$$N_0^2 = 1 + \tfrac{1}{9}v^2l^2(1+k^2) + \mathrm{O}(v^4), \tag{20}$$

$$N_1^2 = \frac{1}{k\sqrt{3}}[1 + \tfrac{2}{25}v^2l^2(1+k^2) + \mathrm{O}(v^4)]. \tag{21}$$

In the eigenvalue equation (4) for eigenfunction selp_1^0 we may put $\gamma = K, \beta = K + iK'$. This gives, using (19),

$$\begin{aligned} N_1^2\, \mathrm{s}\lambda_1^0\, \mathrm{selp}_1^0(K+iK', K) &= \frac{ik^2}{8\pi}\iint_S (\mathrm{sn}^2\gamma' - \mathrm{sn}^2\beta')\, e^{vlk^2 \mathrm{sn}\,\alpha\, \mathrm{sn}\,\beta'\, \mathrm{sn}\,\gamma'} N_1^2\, \mathrm{selp}_1^0(\beta',\gamma')\, d\beta'\, d\gamma' \\ &= \frac{ik^2}{8\pi}\iint_S (\mathrm{sn}^2\gamma' - \mathrm{sn}^2\beta')[vlk^2\, \mathrm{sn}\,\alpha\, \mathrm{sn}^2\beta'\, \mathrm{sn}^2\gamma' \\ &\quad + \tfrac{1}{10}v^3l^3k^4\, \mathrm{sn}\,\alpha\, \mathrm{sn}^2\beta'\, \mathrm{sn}^2\gamma'(\mathrm{sn}^2\beta' + \mathrm{sn}^2\gamma') \\ &\quad + \tfrac{1}{6}v^3l^3k^6\, \mathrm{sn}^3\alpha\, \mathrm{sn}^4\beta'\, \mathrm{sn}^4\gamma']\, d\beta'\, d\gamma' + \mathrm{O}(v^4). \end{aligned} \tag{22}$$

The left-hand side of (22) may be determined using (19) and (21) but the right-hand side requires the evaluation of several lengthy and extremely tedious integrals. It seems not worthwhile to give details of these here, but in an appendix we indicate the technique used and evaluate as an example the contribution coming from the first term of the integrand of (22); a reader interested in further details will find helpful the monograph of Byrd and Friedman (1971). The result for (22) is, to errors of $\mathrm{O}(v^4)$,

$$\mathrm{s}\lambda_1^0[1 + \tfrac{1}{10}(1+k^2)v^2l^2]/k = \tfrac{1}{3}vl\, \mathrm{sn}\,\alpha + v^3l^3[\tfrac{2}{75}(1+k^2)\, \mathrm{sn}\,\alpha + \tfrac{1}{30}k^2\, \mathrm{sn}^2\alpha],$$

and so

$$\mathrm{s}\lambda_1^0 = \tfrac{1}{3}vlk\, \mathrm{sn}\,\alpha\{1 + v^2l^2[\tfrac{1}{10}k^2\, \mathrm{sn}^2\alpha - \tfrac{1}{50}(1+k^2)] + \mathrm{O}(v^4)\}. \tag{23}$$

This is the required expansion for the eigenvalue.

In equation (7) for $\langle x_j x_{j+r}\rangle$ the integral associated with $\mathrm{s}\lambda_1^0$ is I_1^0. If we make use of (18) and (19) we have to order v^2

$$\begin{aligned} N_0^2N_1^2I_1^0 &= \frac{ik^2}{8\pi}\iint_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)k\, \mathrm{sn}^2\beta\, \mathrm{sn}^2\gamma[1 + \tfrac{1}{10}v^2l^2k^2(\mathrm{sn}^2\beta + \mathrm{sn}^2\gamma)] \\ &\quad \times [1 + \tfrac{1}{6}v^2l^2k^2(\mathrm{sn}^2\beta + \mathrm{sn}^2\gamma)]\, d\beta\, d\gamma \\ &= \frac{1}{3k}[1 + \tfrac{16}{75}(1+k^2)v^2l^2], \end{aligned}$$

whence by (20), (21)

$$I_1^0 = \frac{1}{\sqrt{3}}[1+\tfrac{1}{45}(1+k^2)v^2l^2+O(v^4)]. \tag{24}$$

Here again we have omitted details of the integration.

To lowest orders the expression $(I_1^0)^2$ ought to be equal to $\langle x^2\rangle$; this can be checked directly from (13) which after a series expansion and the usual integration yields

$$\langle x^2\rangle = \tfrac{1}{3}[1+\tfrac{2}{45}(1+k^2)v^2l^2+O(v^4)] \tag{25}$$

which is indeed the square of (24). The fact that $\langle x^2\rangle-(I_1^0)^2 = O(v^4)$ is also useful in estimating the infinite series in (7) for we may now write

$$\langle x_j x_{j+r}\rangle = \left(\frac{s\lambda_1^0}{\lambda_0}\right)^r [(I_1^0)^2+R], \tag{26}$$

where

$$R = \sum_{n=1}^{\infty}\sum_{m=0}^{\infty}\left(\frac{s\lambda_{2n+1}^m}{s\lambda_1^0}\right)^r (I_{2n+1}^m)^2$$

$$< \sum_{n=1}^{\infty}\sum_{m=0}^{\infty}(I_{2n+1}^m)^2 = \langle x^2\rangle-(I_1^0)^2 = O(v^4).$$

An expression for λ_0 was already obtained for the calculation of the partition function (Rae 1974), namely

$$\lambda_0 = 1+v^2l^2[\tfrac{1}{6}k^2\,\mathrm{sn}^2\alpha-\tfrac{1}{18}(1+k^2)]+O(v^4). \tag{27}$$

The results (27), (24) and (23) give us explicit forms for all the components of (26) so we have finally

$$\langle x_j x_{j+r}\rangle = \left[\tfrac{1}{3}vlk\,\mathrm{sn}\,\alpha\left(1-\frac{v^2l^2k^2\,\mathrm{sn}^2\alpha}{15}+\frac{8v^2l^2(1+k^2)}{9.25}+O(v^4)\right)\right]^r$$
$$\times\tfrac{1}{3}[1+\tfrac{2}{45}v^2l^2(1+k^2)+O(v^4)]. \tag{28}$$

This expression is of the form expected with exponential fall off for fixed (small) values of v and large r. At the cost of some extremely laborious calculations the higher-order corrections to (28) could be evaluated in a straightforward way.

4. $\langle y_j y_{j+r}\rangle$, $\langle z_j z_{j+r}\rangle$ and susceptibilities at high temperatures

The calculations for the correlation functions $\langle y_j y_{j+r}\rangle$ and $\langle z_j z_{j+r}\rangle$ follow closely on those given above for $\langle x_j x_{j+r}\rangle$ and so will be sketched only in outline.

The ellipsoidal wavefunction cel_1^0 (Arcott 1956), properly normalized, is given by

$$\mathrm{cel}_1^0(z) = \left(\frac{ik\sqrt{3}}{k_1}\right)^{1/2}\mathrm{cn}\,z[1+\tfrac{1}{10}v^2l^2k^2\,\mathrm{sn}^2z-\tfrac{1}{50}v^2l^2(k^2+2)+O(v^4)]. \tag{29}$$

This along with (18) allows the calculation of the integral J_1^0 given by (10) with the result

$$J_1^0 = \frac{1}{\sqrt{3}}\left(1+\frac{v^2l^2(1-2k^2)}{5.9}+O(v^4)\right),$$

and again as a check we may show $\langle y^2\rangle - (J_1^0)^2 = O(v^4)$. The eigenvalue $c\lambda_1^0$ is best obtained by putting $\gamma = 0, \beta = K + iK'$ in its eigenvalue equation (4) to obtain

$$c\lambda_1^0 \operatorname{celp}_1^0(K+iK', 0)$$
$$= \frac{ik^2}{8\pi} \iint_S (\operatorname{sn}^2\gamma' - \operatorname{sn}^2\beta') \exp\left(-\frac{vlk^2}{k_1} \operatorname{cn}\alpha \operatorname{cn}\beta' \operatorname{cn}\gamma'\right) \operatorname{celp}_1^0(\beta'\gamma')\, d\beta'\, d\gamma'.$$

The calculation now proceeds as with (22) and evaluation of the various integrals leads to

$$c\lambda_1^0 = \frac{ikvl \operatorname{cn}\alpha}{3}\left(1 + \frac{v^2l^2(2k^2-1)}{50} - \frac{v^2l^2k^2 \operatorname{cn}^2\alpha}{10} + O(v^4)\right). \tag{30}$$

In order that the interaction strengths a, b, c may take real values with all possible combinations of signs the parameter α must lie in the complex z-plane on the lines $\operatorname{Im} z = \pm K'$. It follows that $i \operatorname{cn}\alpha$ is real so $c\lambda_1^0$ is real as is required. The y–y correlation function is now obtained as

$$\langle y_j y_{j+r}\rangle = \left(\frac{c\lambda_1^0}{\lambda_0}\right)^r [(J_1^0)^2 + O(v^4)]$$
$$= \left[\frac{ivlk \operatorname{cn}\alpha}{3}\left(1 + \frac{v^2l^2k^2\operatorname{cn}^2\alpha}{15} + \frac{8}{9.25}v^2l^2(1-2k^2) + O(v^4)\right)\right]^r$$
$$\times \tfrac{1}{3}[1 + \tfrac{2}{45}v^2l^2(1-2k^2) + O(v^4)]. \tag{31}$$

The calculation for $\langle z_j z_{j+r}\rangle$ follows a similar pattern. The normalized ellipsoidal wavefunction

$$\operatorname{del}_1^0(z) = \left(\frac{\sqrt{3}}{k_1}\right)^{1/2} \operatorname{dn} z[1 + \tfrac{1}{10}v^2l^2k^2 \operatorname{sn}^2 z - \tfrac{1}{50}v^2l^2(1+2k^2) + O(v^4)] \tag{32}$$

is used in the same way as before to calculate the integral K_1^0 as given by (12) with $n = m = 0$. The result is

$$K_1^0 = \frac{1}{\sqrt{3}}\left(1 - \frac{v^2l^2(2-k^2)}{45} + O(v^4)\right). \tag{33}$$

The appropriate eigenvalue $d\lambda_1^0$ is in this case obtained by choosing $\gamma = 0, \beta = K$ in the eigenvalue equation to obtain

$$d\lambda_1^0 \operatorname{delp}_1^0(K, 0)$$
$$= \frac{ik^2}{8\pi} \iint_S (\operatorname{sn}^2\gamma' - \operatorname{sn}^2\beta') \exp\left(\frac{ivl}{k_1} \operatorname{dn}\alpha \operatorname{dn}\beta' \operatorname{dn}\gamma'\right) \operatorname{delp}_1^0(\beta', \gamma')\, d\beta'\, d\gamma'.$$

When this is expanded as a series in v and integrated it yields for the eigenvalue

$$d\lambda_1^0 = \frac{ivl \operatorname{dn}\alpha}{3}(1 - \tfrac{1}{10}v^2l^2 \operatorname{dn}^2\alpha + \tfrac{1}{50}v^2l^2(2-k^2) + O(v^4)]. \tag{34}$$

Following the remarks made after equation (30), the quantity i dn α is real and therefore so is the eigenvalue. The z–z correlation function can now be written as

$$\langle z_j z_{j+r}\rangle = \left(\frac{\mathrm{d}\lambda_1^0}{\lambda_0}\right)^r [(K_1^0)^2 + \mathrm{O}(v^4)]$$

$$= \left[\frac{\mathrm{i}vl\,\mathrm{dn}\,\alpha}{3}\left(1+\frac{v^2l^2\,\mathrm{dn}^2\alpha}{15}+\frac{8}{9\,.\,25}v^2l^2(k^2-2)+\mathrm{O}(v^4)\right)\right]^r$$

$$\times \tfrac{1}{3}[1-\tfrac{2}{45}v^2l^2(2-k^2)+\mathrm{O}(v^4)]. \tag{35}$$

If to the system described by Hamiltonian (1) we add an external magnetic field the model becomes insoluble. Even the partition function has so far defied calculation and so cannot be used to determine susceptibilities. The latter can however be obtained from the correlation functions through the well-known fluctuation–dissipation theorem (see for example Stanley 1971). For the susceptibility in the x direction we have

$$\chi_x = \lim_{N\to\infty}\frac{1}{Nk_\mathrm{B}T}\sum_{i=1}^{N}\sum_{j=1}^{N}\langle x_i x_j\rangle = v\langle x^2\rangle + 2v\sum_{r=1}^{\infty}\langle x_i x_{i+r}\rangle.$$

By substituting (7) in this and performing the sum over r we obtain

$$\chi_x = v\sum_{n=0}^{\infty}\sum_{m=0}^{n}\frac{\lambda_0+\mathrm{s}\lambda_{2n+1}^m}{\lambda_0-\mathrm{s}\lambda_{2n+1}^m}[I_{2n+1}^m]^2$$

and by estimating the infinite series in the manner used in equation (26) we are led to

$$\chi_x = v\frac{\lambda_0+\mathrm{s}\lambda_1^0}{\lambda_0-\mathrm{s}\lambda_1^0}[(I_1^0)^2+\mathrm{O}(v^4)]. \tag{36}$$

In (23), (24) and (27) we have at hand all the contributions to this formula. The final result is

$$\chi_x = \tfrac{1}{3}v[1+\tfrac{2}{3}vlk\,\mathrm{sn}\,\alpha+\tfrac{2}{9}v^2l^2k^2\,\mathrm{sn}^2\,\alpha+\tfrac{2}{45}v^2l^2(1+k^2)+\tfrac{4}{135}v^3l^3k^3\,\mathrm{sn}^3\alpha$$

$$+\tfrac{4}{75}v^3l^3k(1+k^2)\,\mathrm{sn}\,\alpha+\mathrm{O}(v^4)]. \tag{37}$$

The susceptibilities in the y and z directions are also given by formulae of the same structure as (36) but utilizing $\mathrm{c}\lambda_1^0$, J_1^0 and $\mathrm{d}\lambda_1^0$, K_1^0 respectively. The final results for these are

$$\chi_y = \tfrac{1}{3}v[1+\tfrac{2}{3}\mathrm{i}vlk\,\mathrm{cn}\,\alpha-\tfrac{2}{9}v^2l^2k^2\,\mathrm{cn}^2\alpha+\tfrac{2}{45}v^2l^2(1-2k^2)-\tfrac{4}{135}\mathrm{i}v^3l^3k^3\,\mathrm{cn}^3\alpha$$

$$+\tfrac{4}{75}\mathrm{i}v^3l^3k(1-2k^2)\,\mathrm{cn}\,\alpha+\mathrm{O}(v^4)] \tag{38}$$

$$\chi_z = \tfrac{1}{3}v[1+\tfrac{2}{3}\mathrm{i}vl\,\mathrm{dn}\,\alpha-\tfrac{2}{9}v^2l^2\,\mathrm{dn}^2\alpha+\tfrac{2}{45}v^2l^2(k^2-2)-\tfrac{4}{135}\mathrm{i}v^3l^3\,\mathrm{dn}^3\alpha$$

$$+\tfrac{4}{75}\mathrm{i}v^3l^3(k^2-2)\,\mathrm{dn}\,\alpha+\mathrm{O}(v^4)]. \tag{39}$$

5. Conclusions

It has been shown in the preceding sections that exact expressions may be obtained in terms of ellipsoidal wavefunctions for pair correlation functions and susceptibilities of the anisotropic classical Heisenberg model. Explicit high temperature expansions are comparatively straightforward to obtain and are given up to $\mathrm{O}(T^{-4})$ in §§ 3 and 4.

Corresponding results for low temperatures are much more difficult to obtain; an attempt for this limiting case is presented in the companion paper to this one.

The final formulae given in this paper are still rather complicated and in view of the extremely lengthy calculations involved, though not presented explicitly in this article, it is as well to make some check on their validity. For the correlation functions this can be done by using them to calculate $\langle H\rangle$, a quantity which can be found independently from the partition function. We have from (1)

$$-\frac{\langle H\rangle}{N} = a\langle x_i x_{i+1}\rangle + b\langle y_i y_{i+1}\rangle + c\langle z_i z_{i+1}\rangle$$

and on substituting from (3), (28), (31) and (35),

$$-\frac{\langle H\rangle}{N} = \frac{\nu}{3}k^2 l^2 \operatorname{sn}^2\alpha - \frac{\nu l^2}{9}(1+k^2) + \nu^3 l^2\left(-\frac{l^2 k^4 \operatorname{sn}^4\alpha}{45} + \frac{2l^2 k^2(1+k^2)\operatorname{sn}^2\alpha}{135} + \frac{l^2(7k^4-12k^2+7)}{675}\right). \tag{40}$$

But the left-hand side of (40) is related to the partition function Z by

$$-\frac{\langle H\rangle}{N} = \frac{1}{N}\frac{\partial}{\partial \nu}\ln Z = \frac{1}{\lambda_0}\frac{\partial \lambda_0}{\partial \nu}$$

and if we calculate this using the value of λ_0 given in Rae (1974) it agrees exactly with the right-hand side of (40).

Finally we look at some limiting cases. In order to make two of the interaction strengths a, b, c equal it is necessary to take the parameter k as 0 or 1 and it has already been shown that in these cases the ellipsoidal wavefunctions become spheroidal functions (Sleeman 1967, Rae 1974). In this case our formulae such as (9) and (36) reduce to formulae given by Joyce (1967) and Thompson (1968). More explicitly, if we look at the case $b = c = 0, a = J$ corresponding to $k \to 1, \alpha \to \infty + \mathrm{i}K', l = J$ we have to put the latter values into formulae (28) and (37) which immediately reduce to the corresponding formulae given by Thompson (1968). In order to obtain the fully isotropic case $a = b = c = J$ it is necessary to let $\alpha = \mathrm{i}K' + u, l = Ju$ with u real and then take the limit $u \to 0$. Each of the correlation functions (28), (31) and (35) then becomes

$$\left[\frac{1}{3}\nu J\left(1 - \frac{\nu^2 J^2}{15} + \mathrm{O}(\nu^4)\right)\right]^r [\tfrac{1}{3} + \mathrm{O}(\nu^4)]$$

and each of the susceptibilities becomes

$$\tfrac{1}{3}\nu[1 + \tfrac{2}{3}\nu J + \tfrac{2}{9}\nu^2 J^2 + \tfrac{4}{135}\nu^3 J^3 + \mathrm{O}(\nu^4)].$$

These expressions are in complete accord with the results derived for the isotropic Heisenberg model (Fisher 1964).

Appendix. Evaluation of integrals

The results obtained in §§ 3 and 4 depend on the evaluation of many integrals of Jacobian elliptic functions. In this appendix we indicate the method used and evaluate as an example the contribution from the first term of (22).

The technique used is to reduce all the integrals in this article to combinations of the two standard forms:

$$\mathscr{I}_{2n} = \int_{-2K}^{2K} \mathrm{sn}^{2n}z\,\mathrm{d}z, \qquad \mathscr{I}'_{2n} = \int_{K-2\mathrm{i}K'}^{K+2\mathrm{i}K'} \mathrm{sn}^{2n}z\,\mathrm{d}z.$$

For these integrals there are available recurrence formulae (Byrd and Friedman 1971, Arscott 1956):

$$(n+1)k^2\mathscr{I}_{n+2} - n(1+k^2)\mathscr{I}_n + (n-1)\mathscr{I}_{n-2} = 0,$$

and the same for $\mathscr{I}'$, which permit all the integrals to be expressed in terms of those with $n = 0$ and $n = 2$. The last mentioned integrals take the values

$$\mathscr{I}_0 = 4K, \qquad \mathscr{I}'_0 = 4\mathrm{i}K', \qquad \mathscr{I}_2 = \frac{4(K-E)}{k^2}, \qquad \mathscr{I}'_2 = \frac{4\mathrm{i}E'}{k^2},$$

where K, K' and E, E' are the usual complete elliptic integrals of the first and second kinds. A systematic use of the above technique allows all our integrals to be calculated.

As an example we calculate the first term on the right-hand side of equation (22) which leads to the following integral:

$$\frac{\mathrm{i}k^2}{8\pi}\iint_S (\mathrm{sn}^2\gamma' - \mathrm{sn}^2\beta')\,\mathrm{sn}^2\beta'\,\mathrm{sn}^2\gamma'\,\mathrm{d}\beta'\,\mathrm{d}\gamma'$$

$$= \frac{\mathrm{i}k^2}{8\pi}(\mathscr{I}_4\mathscr{I}'_2 - \mathscr{I}_2\mathscr{I}'_4)$$

$$= \frac{\mathrm{i}k^2}{8\pi}\left(\frac{16\mathrm{i}E'}{3k^6}[2(1+k^2)(K-E) - k^2K] - \frac{16\mathrm{i}(K-E)}{3k^6}[2(1+k^2)E' - k^2K']\right)$$

$$= -\frac{2}{3\pi k^2}(KK' - EK' - KE') = \frac{1}{3k^2}.$$

In the last step we used Legendre's relation $EK' + E'K - KK' = \pi/2$.

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