Correlation functions of the classical Heisenberg model. II. Low temperature behaviour

1975 J. Phys. A: Math. Gen. 8 357

(http://iopscience.iop.org/0305-4470/8/3/009)

J. Phys. A: Math. Gen., Vol. 8, No. 3, 1975. Printed in Great Britain. © 1975

Correlation functions of the classical Heisenberg model II. Low temperature behaviour

J Rae†

Department of Physics, Queen Mary College, Mile End Road, London E1 4NS, UK

Received 13 September 1974

Abstract. In the first of this pair of papers exact expressions were obtained for the pair correlation functions and susceptibilities of the classical Heisenberg model in terms of ellipsoidal wavefunctions. Here we examine the low temperature behaviour of these quantities. This necessitates an asymptotic expression for the ellipsoidal functions and, as no suitable form exists in the literature, about half of the present article is used in deriving one. The derivation follows the method of Langer and is to leading order only. This asymptotic form allows explicit calculation of the eigenvalues of the transfer matrix (to leading order) and hence a discussion of the low temperature behaviour of the correlation functions and susceptibilities.

1. Introduction

In the first of this pair of papers (Rae 1975, to be referred to as I) the pair correlation functions and susceptibilities for the anisotropic classical Heisenberg model were expressed in terms of ellipsoidal wavefunctions. In I the behaviour of these quantities for high temperatures was made explicit by means of known series expansions for el functions, series which converge for high enough temperature. For low temperatures, in view of known results for similar models, we can hope only for asymptotic series and these will have to be based on asymptotic expansions of ellipsoidal wavefunctions.

The el functions satisfy the differential equation (Arscott 1964)

$$\frac{d^2f}{dz^2}-(A+Bk^2\,\mathrm{sn}^2z+\mu^2k^4\,\mathrm{sn}^4z)f = 0 \tag{1}$$

where in the context of the Heisenberg model μ is related to temperature by $\mu = vl = l/k_BT$ (see I and Rae 1974) and A and B are μ-dependent eigenvalues. The doubly periodic solutions of (1) are the ellipsoidal wavefunctions, denoted by the generic symbols $\mathrm{el}(z)$ or $\mathrm{el}_n^m(z)$, which are all of the form

$$\mathrm{el}(z) = \mathrm{sn}^\rho z\,\mathrm{cn}^\sigma z\,\mathrm{dn}^\tau z\,F(\mathrm{sn}^2z) \tag{2}$$

with each of ρ, σ, τ being either zero or one and F an entire function of its argument. The el functions therefore fall into eight types according to periodicity and parity and are further labelled by the indices n, m (Arscott 1964, Rae 1974).

There already exist in the literature several asymptotic expansions for el functions. In a series of articles Müller (1966) developed asymptotic expansions for solutions of

† Present address: Theoretical Physics Division, AERE Harwell, Didcot, Oxon.

(1) but these are obtained for large values of B with μ remaining a free parameter and so are inappropriate for our purposes. A more relevant type of expansion has been obtained by Malurkar (1935) and Arscott and Sleeman (1970) by the Horn–Jeffreys technique. This gives a solution of (1) suitable for large values of μ and with properly determined eigenvalues A and B; unfortunately the series so obtained are not uniform and Stokes's phenomenon occurs at the transition points. The calculation of the correlation functions involves many integrals of el functions. It turns out, as will be seen later, that the dominant contributions to these integrals for low temperatures come from the neighbourhoods of the transition points, the very places where the non-uniform series break down. A naive substitution of these series simply leads to divergent integrals. It seems, therefore, that although some portions of Arscott and Sleeman's work are useful to us in what follows, their asymptotic expansions, as they stand, are not helpful in finding the correlation functions.

It is clear from the above that what are needed are uniform asymptotic expansions valid, in particular, at the transition points of (1). Methods for finding such expansions are available in the mathematical literature. The equation (1), however, has the additional slight complication that its transition points are not simple, but double zeros of the leading coefficient. The most suitable method for problems of this type appears to be that of Langer (1934) and we shall adopt his approach.

In § 2 below we calculate suitable uniform expansions for el functions. With appropriate expansions for the eigenvalues A and B the transition points are found to be $z = K, K+iK'$ and their equivalents by periodicity; Langer's method, after a lengthy calculation, yields expansions valid in open regions containing these points. We have had to restrict the present calculation to the leading order in $1/\mu$; the reader will appreciate from what follows that the calculation of corrections, while possible in principle, could only be undertaken as part of a major study of ellipsoidal wavefunctions. The asymptotic forms, being obtained from a linear differential equation, require to be normalized but this can be done without great difficulty as the expressions are uniform in the variable z near transition points. The normalization calculation is presented separately in § 3 as the technique used in performing the integrals recurs throughout this article. The following section considers the calculation of the asymptotic eigenvalues of the transfer matrix, the main ingredient in the correlation functions. Finally, in § 5, we are able to return to the correlation functions and susceptibilities and examine their low temperature behaviour by using the asymptotic formulae in conjunction with the exact expressions obtained in I.

2. Asymptotic expansions for el functions

As observed above the second order differential equation (1) has transition points of second order. A general theory of asymptotic solutions of equations of this type was developed long ago by Langer (1934) and it is this theory which we will follow here.

The solutions of (1) which are of relevance for our problem are the doubly periodic ellipsoidal wavefunctions; these exist only when A and B take special μ-dependent eigenvalues so we must first of all find suitable asymptotic expansions for these values of A and B in powers of μ^{-1}. This preliminary work has already been done by Arscott and Sleeman (1970) and their results, with corrections for a minor misprint, give

$$A \sim k^2\mu^2 + C\mu + O(1) \qquad B \sim -(1+k^2)\mu^2 + D\mu + O(1) \tag{3}$$

where C, D are constants related to the type and indices of the corresponding el function

$$C = -4(\tilde{\beta}+\tilde{\alpha}k)k \qquad D = 4(\tilde{\alpha}+\tilde{\beta}k) \tag{4}$$

with

$$\tilde{\alpha} = n-m+\frac{2-(-1)^{\tau}}{4} \qquad \tilde{\beta} = m+\frac{2-(-1)^{\sigma}}{4}. \tag{5}$$

It follows that the equation (1) can be put into Langer's form

$$\frac{d^2 f}{dz^2}-(\mu^2 q_0(z)+\mu q_1(z)+q_2(z,\mu))f = 0 \tag{6}$$

where

$$\begin{aligned} q_0(z) &= k^2(1-\mathrm{sn}^2 z)(1-k^2\,\mathrm{sn}^2 z) \\ q_1(z) &= C+Dk^2\,\mathrm{sn}^2 z \end{aligned} \tag{7}$$

and

$$q_2(z,\mu) = O(1).$$

The transition points are the zeros of q_0, namely double zeros at $z = K$, $z = K+\mathrm{i}K'$ and points equivalent to these by periodicity.

In order to follow Langer's method we restrict ourselves first of all to z in a neighbourhood of the real interval $[0, K]$ which contains no transition point other than K. We arrange that this transition point lies at the origin by the change of variable $x = K-z$. The equation (6) now becomes

$$\frac{d^2 f}{dx^2}-(\mu^2\chi_0^2(x)+\mu\chi_1(x)+\chi_2(x,\mu))f = 0 \tag{8}$$

with

$$\begin{aligned} \chi_0(x) &= kk_1^2\,\mathrm{sd}\,x\,\mathrm{nd}\,x \\ \chi_1(x) &= C+Dk^2\,\mathrm{cd}^2 x \\ \chi_2(x,\mu) &= O(1) \qquad \text{and} \qquad k_1^2 = 1-k^2. \end{aligned} \tag{9}$$

The essence of Langer's method is to define certain auxiliary quantities by the complicated sequence of formulae

$$\kappa = -\frac{\chi_1(0)}{4\chi_0'(0)} \qquad \eta(x) = \frac{\chi_1(x)}{\chi_0(x)}+\frac{2\kappa\chi_0(x)}{\int_0^x \chi_0(x)\,dx} \tag{10a, b}$$

$$\phi(x) = 2\chi_0(x)+\frac{1}{\mu}\eta(x) \qquad \Phi(x) = \int_0^x \phi(x)\,dx \tag{10c, d}$$

$$\xi = \mu\Phi(x) \qquad \Psi(x) = \frac{\Phi^{1/4}(x)}{\phi^{1/2}(x)} \tag{10e, f}$$

and observe that the functions

$$y_{\pm}(x) = \Psi(x)\xi^{-1/4}W_{\pm\kappa,1/4}(\pm\xi) \tag{11}$$

where W is the Whittaker function (Abramowitz and Stegun 1965, Whittaker and Watson 1965) satisfy the differential equation

$$\frac{d^2y}{dx^2}-(\mu^2\chi_0^2(x)+\mu\chi_1(x)+\Omega(x,\mu))y = 0 \tag{12}$$

with $\Omega(x,\mu) = O(1)$. Comparison with equation (8) shows that to leading orders the functions $y_\pm$ satisfy the ellipsoidal wave equation: in fact Langer's paper shows that the corrections are $O(1/\mu)$, that is to each function y of (11) there corresponds a solution f of (8) with $f-y = O(1/\mu)$. Langer actually uses Whittaker's M function instead of W but the latter is more convenient here.

We now have the problem of carrying through the sequence of transformations (10) for our particular case, that is starting from (9). It is easy to see that

$$\kappa = \tilde{\beta} \qquad \int_0^x \chi_0(x)\,dx = k(1-\text{cd}\,x) \tag{13}$$

and with help from tables of integrals of elliptic functions (eg, Byrd and Friedman 1971)

$$\int_\epsilon^x \frac{\chi_1(x')}{\chi_0(x')}\,dx' = \int_\epsilon^x \frac{C+Dk^2\,\text{cd}^2x'}{kk_1^2\,\text{sd}\,x'\,\text{nd}\,x'}\,dx' = \ln\left[\left(\frac{\text{cn}\,x'+\text{dn}\,x'}{\text{sn}\,x'}\right)^{4\beta}\left(\frac{\text{dn}\,x'+k\,\text{cn}\,x'}{k_1}\right)^{4\tilde{a}}\right]_\epsilon^x \tag{14}$$

and

$$\int_\epsilon^x \chi_0(x')\left(\int_0^{x'}\chi_0(x'')\,dx''\right)^{-1}dx' = \ln\left[\int_0^{x'}\chi_0(x'')\,dx''\right]_\epsilon^x = \ln[k-k\,\text{cd}\,x']_\epsilon^x. \tag{15}$$

These results together with formulae (10) enable us to calculate Langer's fundamental variable ξ:

$$\xi = 2k\mu(1-\text{cd}\,x)+\ln\left[\left(\frac{\text{dn}\,x+k\,\text{cn}\,x}{1+k}\right)^{4\tilde{a}}\left(\frac{\text{cn}\,x+\text{dn}\,x}{\text{sn}\,x}\right)^{4\tilde{\beta}}\left(\frac{1-\text{cd}\,x}{2k_1^2}\right)^{2\tilde{\beta}}\right]. \tag{16}$$

Note that as $x\to 0$, $\xi\to 0$ like x^2 so that the mapping from ξ to x is two-valued. If we are interested in only the leading order in $1/\mu$ the prefactor in (11) may be taken as

$$\Psi(x)\xi^{-1/4} = \frac{1}{\mu^{1/4}\phi^{1/2}(x)} \sim \frac{1}{2^{1/2}\mu^{1/4}\chi_0^{1/2}(x)}. \tag{17}$$

Since the functions (11) are linearly independent solutions of (12) it follows that to leading order the ellipsoidal wavefunctions are suitable linear combinations of

$$\chi_0^{-1/2}(x)W_{\pm\tilde{\beta},1/4}(\pm\xi) \tag{18}$$

with $\chi_0(x)$ given by (9) and ξ by (16).

The particular linear combination of (18) which corresponds to a given standard el function depends on the type of the latter and may be determined by parity arguments in the style of Arscott and Sleeman (1970) as follows. For nonzero fixed x and μ large,

ξ is large. We may use the well-known asymptotic expansion for Whittaker functions (Whittaker and Watson 1965) to approximate (18) by

$$\chi_0^{-1/2}(x)\, e^{\mp 1/2\xi}\xi^{\pm\tilde{\beta}}(1+O(1/\xi)).$$

On using (16) and reverting to the original variable $z = K-x$ we find this is equal to leading order to

$$f^{\pm} = N_{\pm}\, e^{\pm k\mu\, \mathrm{sn}\, z}(\mathrm{cn}\, z)^{-\frac{1}{2}-2\tilde{\beta}}(\mathrm{dn}\, z)^{-\frac{1}{2}-2\tilde{\alpha}}(1\mp \mathrm{sn}\, z)^{2\tilde{\beta}}(1\mp k\, \mathrm{sn}\, z)^{2\tilde{\alpha}} \tag{19}$$

where

$$N_{\pm} = e^{\mp k\mu}\frac{1}{k^{1/2}k_1}\left(\frac{1-k}{1+k}\right)^{\pm\tilde{\alpha}}(4k\mu)^{\pm\tilde{\beta}}.$$

The expression (19), which is valid away from $z = K$, is the result obtained with the Horn–Jeffreys method by Malurkar (1935) and Arscott and Sleeman (1970) (with their minor misprints corrected). On changing z to $-z$ the solution f^{+} of (19) goes to $(N_{+}/N_{-})f^{-}$. It follows that el functions with even parity at $z = 0$ must be proportional to the linear combination

$$N_{-}f^{+}+N_{+}f^{-} \tag{20}$$

and those with odd parity to

$$N_{-}f^{+}-N_{+}f^{-}. \tag{21}$$

This gives us at once that, up to a normalization factor, the ellipsoidal wavefunctions uel, cel, del may be approximated uniformly by

$$\chi_0^{-1/2}(x)(N_{-}W_{\tilde{\beta},1/4}(\xi)+N_{+}W_{-\tilde{\beta},1/4}(-\xi)) \tag{22}$$

and sel is given by the corresponding expression with a minus sign between the terms. The normalization of (22) will be discussed later.

The above discussion applies for z in a region containing $z = K$ and no other transition point; we next look at the behaviour around $z = K+iK'$. An appropriate change of variable now is $z = K+iK'-iy$ which brings the transition point $z = K+iK'$ to $y = 0$. By means of the formula

$$k^2\, \mathrm{sn}^2(z,k) = \mathrm{dn}^2(y,k_1), \qquad k_1^2 = 1-k^2$$

the equation (6) becomes in this case

$$\frac{d^2f}{dy^2}-(\mu^2X_0^2(y)+\mu X_1(y)+X_2(y,\mu))f = 0 \tag{23}$$

with

$$\begin{aligned} X_0(y) &= k_1^2\, \mathrm{sn}(y,k_1)\, \mathrm{cn}(y,k_1) \\ X_1(y) &= -C-D\, \mathrm{dn}^2(y,k_1) \\ X_2(y,\mu) &= O(1). \end{aligned} \tag{24}$$

The previous argument may be worked through once more with the results (here we use ζ in place of ξ)

$$\kappa = \tilde{\alpha} \tag{25}$$

$$\zeta = 2\mu[1-\mathrm{dn}(y,k_1)]+\ln\left[\left(\frac{\mathrm{dn}(y,k_1)+k}{(1+k)\,\mathrm{cn}(y,k_1)}\right)^{4\tilde{\beta}}\left(\frac{1+\mathrm{dn}(y,k_1)}{k_1k^2\, \mathrm{sn}(y,k_1)}\right)^{4\tilde{\alpha}}\left(\frac{1-\mathrm{dn}(y,k_1)}{2}\right)^{2\tilde{\alpha}}\right]. \tag{26}$$

The particular combination of Whittaker functions to be used in this case may be determined by examining the parity at the point $z = K + \mathrm{i}K'$; the conclusion is that all four functions of interest, uel, sel, cel, del are simply proportional to

$$X_0^{-1/2}(y) W_{\tilde{\alpha}, 1/4}(\zeta) \tag{27}$$

where X_0 and ζ are given by the above. If we expand (27) as an asymptotic series for large ζ and revert to the original variable z, the term (27) is proportional to f^+ given by (19) in accordance with the results of the Horn–Jeffreys method.

3. Normalization of ellipsoidal wavefunctions

In this section we normalize the asymptotic expressions we have obtained for the functions uelp, selp, celp and delp. It seems worth discussing this in some detail in a separate section as the type of integrals we will evaluate here will occur throughout the rest of this article.

The normalization to be used here (see I) is

$$\frac{\mathrm{i}k^2}{8\pi} \int\int_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)[\mathrm{elp}(\beta, \gamma)]^2 = 1 \tag{28}$$

which by periodicity arguments may be written

$$\frac{2\mathrm{i}k^2}{\pi} \int_0^K \mathrm{d}\gamma \int_K^{K+\mathrm{i}K'} \mathrm{d}\beta (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)[\mathrm{elp}(\beta, \gamma)]^2 = 1. \tag{29}$$

For $\gamma \in [0, K]$ we may transform to variables x, ξ of § 2 and use formulae of the form (22) for $\mathrm{el}(\gamma)$ according to its type. However, since these formulae are derived for $\mu \to +\infty$ and $\mathrm{sn}\,\gamma \geqslant 0$ for $\gamma \in [0, K]$ it is clear that the contribution coming from $W_{-\tilde{\beta}, 1/4}(-\xi)$ is in all cases exponentially small within the integral (29) and may be neglected. Thus we may take

$$\mathrm{el}(\gamma) = N(\tilde{\beta}) \chi_0^{-1/2}(x) W_{\tilde{\beta}, 1/4}(\xi) \tag{30}$$

where $N(\tilde{\beta})$ is a normalization constant to be determined. Similarly in the range of integration of β we may take

$$\mathrm{el}(\beta) = N(\tilde{\alpha}) X_0^{-1/2}(y) W_{\tilde{\alpha}, 1/4}(\zeta). \tag{31}$$

Having made these substitutions in (29) the integrals are best evaluated in terms of the variables ξ, ζ. Let us look first at

$$I_1 = \int_0^K \mathrm{d}\gamma (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)[\mathrm{el}(\gamma)]^2.$$

From (16), (17) and (9) we have to leading order

$$\mathrm{sn}^2\gamma = \left(1 - \frac{\xi}{2k\mu}\right)^2 \qquad \mathrm{d}\gamma = -\frac{\mathrm{d}\xi}{2\mu\chi(\xi)}$$

$$\chi_0(x) = k\left[\left(\frac{\xi}{k\mu} - \frac{\xi^2}{4k^2\mu^2}\right)\left(k_1^2 + \frac{\kappa\xi}{\mu} - \frac{\xi^2}{4\mu^2}\right)\right]^{1/2} \equiv \chi(\xi) \tag{32}$$

and therefore

$$I_1 = \int_0^{2k\mu} \mathrm{d}\xi \left[\left(1 - \frac{\xi}{2k\mu}\right)^2 - \mathrm{sn}^2\beta \right] \frac{N^2(\tilde{\beta})}{2\mu\chi^2(\xi)} [W_{\tilde{\beta},1/4}(\xi)]^2. \tag{33}$$

We have been working throughout to the leading order in $1/\mu$ so we may to within the same approximation simplify (33) quite considerably. Since the Whittaker function falls off exponentially we may replace the upper limit of integration by $+\infty$ and then expand the remaining part of the integrand in powers of ξ/λ and drop all but the leading term. This gives

$$I_1 = \frac{1}{2kk_1^2} N^2(\tilde{\beta})(1 - \mathrm{sn}^2\beta) \int_0^\infty \xi^{-1} [W_{\tilde{\beta},1/4}(\xi)]^2 \, \mathrm{d}\xi. \tag{34}$$

The remaining integral is standard; it may be found, for example, in Gradshteyn and Ryzhik (1965 formula 7.611(4)), or by expressing the Whittaker function in terms of Hermite polynomials. The result depends, of course, on $\tilde{\beta}$ given by (5) and may in all cases be expressed as $\Gamma(m+1)\Gamma(2\tilde{\beta}-m)$. By using I_1 the normalization integral (29) may be put in the form

$$\frac{2\mathrm{i}k^2}{\pi} \frac{N^2(\tilde{\beta})}{2kk_1^2} \Gamma(m+1)\Gamma(2\tilde{\beta}-m) \int_K^{K+\mathrm{i}K'} (1 - \mathrm{sn}^2\beta)[\mathrm{el}(\beta)]^2 \, \mathrm{d}\beta = 1$$

leading, after corresponding substitutions in the β integral to

$$\frac{\mathrm{i}kN^2(\tilde{\beta})}{\pi k_1^2} \Gamma(m+1)\Gamma(2\beta - m) \frac{(-\mathrm{i})N^2(\tilde{\alpha})}{2k^2} \int_0^\infty \zeta^{-1} [W_{\tilde{\alpha},1/4}(\zeta)]^2 \, \mathrm{d}\zeta = 1. \tag{35}$$

The remaining integral here is the same as in (34); it takes the value

$$\Gamma(n-m+1)\Gamma(2\tilde{\alpha}-n+m).$$

A simple re-arrangement of (35) now gives the normalization constants

$$N^2(\tilde{\alpha})N^2(\tilde{\beta}) = 2\pi kk_1^2 (\Gamma(m+1)\Gamma(n-m+1)\Gamma(2\tilde{\beta}-m)\Gamma(2\tilde{\alpha}-n+m))^{-1}. \tag{36}$$

The normalization condition (28) being a condition on elp only determines this combination of normalizing factors. This, however, is all that is needed in what follows. The method used in this section for evaluating the integrals will be followed closely in the rest of this article.

4. The eigenvalues of the transfer matrix

The eigenvalue equation for the transfer matrix has already been given in equation (4) of I. For the eigenfunctions uelp_{2n}^m it may be written

$$\frac{\mathrm{i}k^2}{8\pi} \int\int_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta) \, \mathrm{e}^{\mu k^2 \mathrm{sn}\,\alpha\, \mathrm{sn}\,\beta\, \mathrm{sn}\,\gamma} \, \mathrm{uelp}_{2n}^m(\beta, \gamma) \, \mathrm{d}\beta \, \mathrm{d}\gamma = \mathrm{u}\lambda_{2n}^m \, \mathrm{uelp}_{2n}^m(K + \mathrm{i}K', K) \tag{37}$$

or, making use of periodicity,

$$\frac{\mathrm{i}k^2}{\pi} \int_0^K \mathrm{d}\gamma \int_K^{K+\mathrm{i}K'} \mathrm{d}\beta (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta) 2\cosh(\mu k^2 \, \mathrm{sn}\,\alpha \, \mathrm{sn}\,\beta \, \mathrm{sn}\,\gamma) \, \mathrm{uelp}_{2n}^m(\beta, \gamma)$$
$$= \mathrm{u}\lambda_{2n}^m \, \mathrm{uelp}_{2n}^m(K + \mathrm{i}K', K). \tag{38}$$

This is now in a form suitable for using the asymptotic formula for uelp. Notice, however, that for consistency we ought then to drop the decreasing exponential term in cosh, that is, we should replace the 2cosh factor by $\exp(\mu k^2|\operatorname{sn}\alpha|\operatorname{sn}\beta\operatorname{sn}\gamma)$ since $\operatorname{sn}\beta$ and $\operatorname{sn}\gamma$ are non-negative in the region of integration. The double integral may now be evaluated by the method used in § 3. To leading order the exponential factor

$$\exp(\mu k^2|\operatorname{sn}\alpha|\operatorname{sn}\beta\operatorname{sn}\gamma) \sim \exp(\mu k|\operatorname{sn}\alpha|)\exp(-\tfrac{1}{2}|\operatorname{sn}\alpha|\xi)\exp(-\tfrac{1}{2}k|\operatorname{sn}\alpha|\zeta) \quad (39)$$

so that the γ integration in (38) may be extracted as

$$I_2 = \int_0^K \mathrm{d}\gamma(\operatorname{sn}^2\gamma-\operatorname{sn}^2\beta)\,\mathrm{e}^{-\frac{1}{2}|\operatorname{sn}\alpha|\xi}\,\mathrm{uel}^m_{2n}(\gamma). \quad (40)$$

(From here on we suppose $\operatorname{sn}\alpha > 0$ for simplicity; for the negative case $\operatorname{sn}\alpha$ should be replaced by $|\operatorname{sn}\alpha|$ throughout.) If we now change completely to the variable ξ, insert the asymptotic formula (30) and keep only the leading order we have

$$\begin{aligned} I_2 &\sim \frac{N(m+\frac{1}{4})(1-\operatorname{sn}^2\beta)}{2\mu^{1/4}k^{3/4}k_1^{3/2}}\int_0^\infty \xi^{-3/4}\,\mathrm{e}^{-\frac{1}{2}\operatorname{sn}\alpha\xi}W_{m+1/4,1/4}(\xi)\,\mathrm{d}\xi \\ &= \frac{N(m+\frac{1}{4})(1-\operatorname{sn}^2\beta)}{2^{2m+1}\mu^{1/4}k^{3/4}k_1^{3/2}}\int_0^\infty \mathrm{e}^{-\frac{1}{2}\xi(1+\operatorname{sn}\alpha)}\xi^{-1/2}H_{2m}(\xi^{1/2})\,\mathrm{d}\xi \\ &= \frac{N(m+\frac{1}{4})(1-\operatorname{sn}^2\beta)}{2^{2m+1}\mu^{1/4}k^{3/4}k_1^{3/2}}\left(\frac{2}{1+\operatorname{sn}\alpha}\right)^{1/2}\left(\frac{1-\operatorname{sn}\alpha}{1+\operatorname{sn}\alpha}\right)^m\frac{(2m)!}{m!}\pi^{1/2}. \end{aligned}$$

For the relationship between the Whittaker function and Hermite polynomial and for the evaluation of the integral see, for example, Abramowitz and Stegun (1965, 13.6.38 and 22.13.17 respectively). This expression for I_2 is now to be put back into (38) and the β integration performed. In terms of the variable ζ of § 2 this amounts to almost the same calculation as that just given for I_2 and so will not be given again. The final result for the left-hand side of (38) is

$$\begin{aligned} &\frac{N(m+\frac{1}{4})N(n-m+\frac{1}{4})}{2^{2n+1}\mu^{1/2}k^{3/4}k_1}\,\frac{\mathrm{e}^{\mu k\operatorname{sn}\alpha}}{(1+\operatorname{sn}\alpha)^{1/2}(1+k\operatorname{sn}\alpha)^{1/2}}\,\frac{(2m)!}{m!}\,\frac{[2(n-m)]!}{(n-m)!} \\ &\qquad\times\left(\frac{1-\operatorname{sn}\alpha}{1+\operatorname{sn}\alpha}\right)^m\left(\frac{1-k\operatorname{sn}\alpha}{1+k\operatorname{sn}\alpha}\right)^{n-m}. \end{aligned} \quad (41)$$

For the right-hand side of (38), $\mathrm{uelp}^m_{2n}(K+\mathrm{i}K', K)$ may be evaluated by direct substitution of $\gamma = K$ in (30) and $\beta = K+\mathrm{i}K'$ in (31). This gives

$$\mathrm{uelp}^m_{2n}(K+\mathrm{i}K', K) \sim (-1)^n\frac{N(m+\frac{1}{4})N(n-m+\frac{1}{4})\mu^{1/2}}{2^{2n}k^{1/4}k_1}\,\frac{(2m)!}{m!}\,\frac{[2(n-m)]!}{(n-m)!}. \quad (42)$$

Finally, if (41) and (42) are used in (38) we obtain the desired asymptotic expression for the eigenvalue

$$\mathrm{u}\lambda^m_{2n} \sim \frac{\mathrm{e}^{\mu k\operatorname{sn}\alpha}}{2\mu(1+k\operatorname{sn}\alpha)^{1/2}(k+k\operatorname{sn}\alpha)^{1/2}}\left(\frac{\operatorname{sn}\alpha-1}{\operatorname{sn}\alpha+1}\right)^m\left(\frac{k\operatorname{sn}\alpha-1}{k\operatorname{sn}\alpha+1}\right)^{n-m}. \quad (43)$$

As the parameter α in the case considered will lie between $\mathrm{i}K'$ and $K+\mathrm{i}K'$ on the line $\operatorname{Im}\alpha = K'$ we have $\operatorname{sn}\alpha > k\operatorname{sn}\alpha > 1$. Thus the expression for $\mathrm{u}\lambda$ is always positive and the last two factors in (43) are of magnitude less than unity. It follows that the maximum $u\lambda$ is given by $n = m = 0$

$$\lambda_0 \equiv u\lambda_0^0 \sim \frac{e^{\mu k \operatorname{sn}\alpha}}{2\mu(1+k\operatorname{sn}\alpha)^{1/2}(k+k\operatorname{sn}\alpha)^{1/2}} \tag{44}$$

in agreement with the expression found in earlier work (Rae 1974).

If we turn now to the eigenvalues $s\lambda_{2n+1}^m$ corresponding to eigenfunctions selp_{2n+1}^m we find that the argument used above can be carried through exactly as before and, indeed, since $\tilde{\alpha}$, $\tilde{\beta}$ are the same for uel_{2n}^m and sel_{2n+1}^m leads to exactly the same expression (43). Further, on looking again at Langer's method it is apparent that even taking into account corrections to this leading term we would obtain *exactly* the same asymptotic series for uel and sel, the differences being $O(e^{-\mu})$. We conclude, then, that to leading order $s\lambda_{2n+1}^m$ is given by (43).

For the eigenvalues $c\lambda_{2n+1}^m$ the discussion has to be changed a little since the functions $\mathrm{cel}(\gamma)$ are zero for $\gamma = K$. The simplest adaptation of the argument is to differentiate the eigenvalue equation with respect to γ before putting $\gamma = K$, $\beta = K+iK'$. This gives

$$c\lambda\, \mathrm{cel}(K+iK')\, \mathrm{cel}'(K)$$
$$= \frac{i\mu k^4 \operatorname{cn}\alpha}{\pi}\int_0^K d\gamma \int_K^{K+iK'} d\beta(\operatorname{sn}^2\gamma-\operatorname{sn}^2\beta)\operatorname{cn}\beta\operatorname{cn}\gamma\, e^{\mu k^2 \operatorname{sn}\alpha\operatorname{sn}\beta\operatorname{sn}\gamma}\,\mathrm{celp}(\beta,\gamma). \tag{45}$$

By direct substitution of $\beta = K+iK'$ in (31) one obtains

$$\mathrm{cel}_{2n+1}^m(K+iK') \sim (-1)^{n-m}\frac{N(n-m+\frac{1}{4})\mu^{1/4}}{2^{2(n-m)}k_1^{1/2}}\frac{[2(n-m)]!}{(n-m)!} \tag{46}$$

and by differentiating (30) with respect to γ and putting $\gamma = K$

$$\mathrm{cel}'^m_{2n+1}(K) \sim (-1)^{m+1}2\mu^{3/4}k^{1/4}k_1^{1/2}\pi^{-1/2}N(m+\tfrac{3}{4})\Gamma(m+\tfrac{3}{2}). \tag{47}$$

The integral on the right-hand side of (45) may be evaluated by the technique already used for (38); there are no noteworthy features except that $\mathrm{cel}_{2n+1}^m(\gamma)$ now appears in terms of $W_{m+3/4,1/4}(\xi)$ and hence in terms of $H_{2m+1}(\xi^{1/2})$ so that it has indeed a simple zero at $\gamma = K$. The result for the eigenvalue is

$$c\lambda_{2n+1}^m \sim \frac{ik\operatorname{cn}\alpha}{2\mu}e^{\mu k\operatorname{sn}\alpha}(k+k\operatorname{sn}\alpha)^{-3/2}(1+k\operatorname{sn}\alpha)^{-1/2}\left(\frac{\operatorname{sn}\alpha-1}{\operatorname{sn}\alpha+1}\right)^m\left(\frac{k\operatorname{sn}\alpha-1}{k\operatorname{sn}\alpha+1}\right)^{n-m}. \tag{48}$$

Note that $i\operatorname{cn}\alpha$ is a real quantity so the eigenvalue is real as is necessary for a Hilbert–Schmidt operator.

Lastly, a similar calculation may be performed for $d\lambda_{2n+1}^m$. In this case it is convenient to differentiate the eigenvalue equation with respect to β and so obtain

$$d\lambda\, \mathrm{del}(K)\, \mathrm{del}'(K+iK')$$
$$= -\frac{i\mu k^2 \operatorname{dn}\alpha}{\pi}\int_0^K d\gamma \int_K^{K+iK'} d\beta(\operatorname{sn}^2\gamma-\operatorname{sn}^2\beta)\operatorname{dn}\beta\operatorname{dn}\gamma\, e^{\mu k^2 \operatorname{sn}\alpha\operatorname{sn}\beta\operatorname{sn}\gamma}\,\mathrm{delp}(\beta,\gamma). \tag{49}$$

Here it is $\mathrm{del}_{2n+1}^m(\beta)$ which is related to the odd Hermite polynomial $H_{2(n-m)+1}(\zeta^{1/2})$ and so has the expected simple zero at $\beta = K+iK'$. The calculation, though lengthy, goes through just as above to yield

$$\mathrm{d}\lambda_{2n+1}^{m} \sim \frac{\mathrm{i}\,\mathrm{dn}\,\alpha}{2\mu}\,\mathrm{e}^{\mu k\,\mathrm{sn}\,\alpha}(k+k\,\mathrm{sn}\,\alpha)^{-1/2}(1+k\,\mathrm{sn}\,\alpha)^{-3/2}\left(\frac{\mathrm{sn}\,\alpha-1}{\mathrm{sn}\,\alpha+1}\right)^{m}\left(\frac{k\,\mathrm{sn}\,\alpha-1}{k\,\mathrm{sn}\,\alpha+1}\right)^{n-m} \tag{50}$$

Here $\mathrm{i}\,\mathrm{dn}\,\alpha$ is real and hence so is the eigenvalue.

The above calculations are so complicated that it is useful to make an independent check of the results. This may be done by using for the kernel $K(\alpha;\beta,\gamma;\beta',\gamma')$ of the transfer matrix (see I, equation (4)) the sum over *all* normalized eigenfunctions and eigenvalues

$$\sum \lambda_n^m\,\mathrm{elp}_n^m(\beta,\gamma)\,\mathrm{elp}_n^m(\beta',\gamma') \tag{51}$$

which comes from the completeness of ellipsoidal surface wavefunctions. If we choose $\gamma=\gamma'=K$, $\beta=\beta'=K+\mathrm{i}K'$ all terms in the sum vanish except those involving uelp or selp. We know from (42), (36) that

$$[\mathrm{uelp}_{2n}^{m}(K+\mathrm{i}K',K)]^2 \sim [\mathrm{selp}_{2n+1}^{m}(K+\mathrm{i}K',K)]^2 \sim \mu k^{1/2}2^{-2n+1}\frac{(2m)!}{(m!)^2}\frac{[2(n-m)]!}{[(n-m)!]^2}$$

and from (43) an asymptotic expression for $\mathrm{u}\lambda_{2n}^{m}$ and $\mathrm{s}\lambda_{2n+1}^{m}$. Inserting these into (51) and putting $n-m=r$ the series becomes

$$\mathrm{e}^{\mu k\,\mathrm{sn}\,\alpha}(1+k\,\mathrm{sn}\,\alpha)^{-1/2}(1+\mathrm{sn}\,\alpha)^{-1/2}2\sum_{m=0}^{\infty}\frac{(2m)!}{2^{2m}(m!)^2}\left(\frac{\mathrm{sn}\,\alpha-1}{\mathrm{sn}\,\alpha+1}\right)^{m}\sum_{r=0}^{\infty}\frac{(2r)!}{2^{2r}(r!)^2}\left(\frac{k\,\mathrm{sn}\,\alpha-1}{k\,\mathrm{sn}\,\alpha+1}\right)^{r}$$
$$= \mathrm{e}^{\mu k\,\mathrm{sn}\,\alpha}$$

which is indeed $K(\alpha;K+\mathrm{i}K',K;K+\mathrm{i}K',K)$ as required. A similar check has been made for cases $\mathrm{c}\lambda$ and $\mathrm{d}\lambda$ by considering $\partial^2K/\partial\gamma\partial\gamma'$ and $\partial^2K/\partial\beta\partial\beta'$; these involve consideration of ellipsoidal functions scel and sdel and will not be reproduced here.

5. The correlation functions and susceptibilities

After the extensive preliminaries of the preceding sections we are now in a position to return to the correlation functions and susceptibilities of the classical Heisenberg model. These quantities were defined in I in terms of ellipsoidal wavefunctions and we may now use the asymptotic expansions of this article to elicit the low temperature behaviour.

For the calculation of $\langle x_j x_{j+r}\rangle$ it is convenient to evaluate first of all the self-correlation $\langle x^2\rangle$. From (30), (31) and I(13) we have

$$\langle x^2\rangle = \frac{\mathrm{i}k^2}{8\pi}\iint_S (\mathrm{sn}^2\gamma-\mathrm{sn}^2\beta)k^2\,\mathrm{sn}^2\beta\,\mathrm{sn}^2\gamma[\mathrm{uelp}_0^0(\beta,\gamma)]^2\,\mathrm{d}\beta\,\mathrm{d}\gamma$$
$$\sim \frac{2\mathrm{i}k^4}{\pi}\int_0^K \mathrm{d}\gamma\int_K^{K+\mathrm{i}K'}\mathrm{d}\beta(\mathrm{sn}^2\gamma-\mathrm{sn}^2\beta)\,\mathrm{sn}^2\beta\,\mathrm{sn}^2\gamma\,N^4(\tfrac{1}{4})\chi^{-1}(\xi)X^{-1}(\zeta)$$
$$\times W^2_{1/4,1/4}(\xi)W^2_{1/4,1/4}(\zeta) \sim 1. \tag{52}$$

In evaluating the integral here we have used again the methods employed in §§ 3 and 4. Since the points $\beta=K+\mathrm{i}K'$, $\gamma=K$ give the dominant contribution we may, in fact, put $\mathrm{sn}\,K=1$ and $\mathrm{sn}(K+\mathrm{i}K')=1/k$ into the integrand and the integral in (52) then reduces precisely to the normalization integral (29). Since sel_1^0 and uel_0^0 have the same asymptotic expansion this argument applies equally to the integral I_1^0 (see I, equation (8)) which is also asymptotically equal to 1. Thus we have for large μ

$$\langle x^2\rangle - (I_1^0)^2 = \mathrm{O}(1/\mu). \tag{53}$$

The asymptotic form of $\langle x_j x_{j+r}\rangle$ depends on the greatest of the eigenvalues $\mathrm{s}\lambda_{2n+1}^m$; from § 4 this is plainly $\mathrm{s}\lambda_1^0$ which has the same asymptotic expansion as λ_0 namely formula (44). (We may note in passing that $\mathrm{s}\lambda_1^0$ was the greatest of the $\mathrm{s}\lambda_{2n+1}^m$ also for high temperatures. It seems likely that this is true throughout the temperature range but I have no proof of this.) We now have, as in I(26)

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

with

$$R < \langle x^2\rangle - (I_1^0)^2 = \mathrm{O}(1/\mu) \tag{54}$$

or

$$\langle x_j x_{j+r}\rangle \sim 1 + \mathrm{O}(1/\mu) \tag{55}$$

and to within errors of $\mathrm{O}(\mathrm{e}^{-\mu})$ there is no r dependence. As the susceptibility χ_x is proportional to $(\lambda_0 + \mathrm{s}\lambda_1^0)/(\lambda_0 - \mathrm{s}\lambda_1^0)$ this shows an exponential $\mathrm{e}^{-1/T}$ type of divergence as $T \to 0$. Similar behaviour was found for the partially anisotropic model by Joyce (1967). It should be noted that the dominant role played by the point $\gamma = K, \beta = K + \mathrm{i}K'$ in the low temperature limit ought to be expected since the x–x coupling a was taken to be of greatest magnitude and by I(3) the point $\gamma = K, \beta = K + \mathrm{i}K'$ corresponds to $x = 1, y = z = 0$.

The corresponding results for the y and z directions, to which we now turn, are somewhat less trivial. From (48) it is clear that the greatest of $\mathrm{c}\lambda_{2n+1}^m$ again corresponds to $n = m = 0$. By using the methods employed earlier, and since $\mathrm{cn}K = 0$ this case is not just a disguised form of the normalization integral, we obtain

$$\langle y^2\rangle = \frac{\mathrm{i}k^2}{8\pi}\int\!\!\int_S (\mathrm{sn}^2\gamma - \mathrm{sn}^2\beta)\left(\frac{-k^2}{k_1^2}\right) \mathrm{cn}^2\beta\, \mathrm{cn}^2\gamma[\mathrm{uelp}_0^0(\beta,\gamma)]^2 \sim 1/(2k\mu) \tag{56}$$

and find that $(J_1^0)^2$ (as given by I(10)) has the same asymptotic limit. Thus we have

$$\langle y^2\rangle - (J_1^0)^2 = \mathrm{O}(1/\mu^2)$$

and the correlation function becomes

$$\langle y_j y_{j+r}\rangle = \left(\frac{\mathrm{c}\lambda_1^0}{\lambda_0}\right)^r ((J_1^0)^2 + \mathrm{O}(1/\mu^2)) = \left[\frac{\mathrm{i}\,\mathrm{cn}\,\alpha}{1+\mathrm{sn}\,\alpha} + \mathrm{O}\left(\frac{1}{\mu}\right)\right]^r \left[\frac{1}{2k\mu} + \mathrm{O}\left(\frac{1}{\mu^2}\right)\right]. \tag{57}$$

Thus for small fixed temperature T the correlation function falls off exponentially with r, and for $T = 0$ it also is zero as it should be since all the y components of the spins vanish. The susceptibility in the y direction is given by (cf I(36))

$$\chi_y = \frac{1}{k_\mathrm{B}T}\left(\frac{\lambda_0 + \mathrm{c}\lambda_1^0}{\lambda_0 - \mathrm{c}\lambda_1^0}\right)((J_1^0)^2 + \mathrm{O}(1/\mu^2))$$

$$\sim \frac{1}{2kl}\,\frac{1+\mathrm{sn}\,\alpha + \mathrm{i}\,\mathrm{cn}\,\alpha}{1+\mathrm{sn}\,\alpha - \mathrm{i}\,\mathrm{cn}\,\alpha} = \frac{1}{2kl}\,\frac{1}{\mathrm{sn}\,\alpha - \mathrm{i}\,\mathrm{cn}\,\alpha} = \frac{1}{2(a-b)}. \tag{58}$$

The last expression is just what one would expect from an elementary calculation. At low temperatures the spins with Hamiltonian I(1) are lined up in the x direction. A weak magnetic field h added in the y direction will rotate each spin in the xy plane by a small angle $\theta = h/2(a-b)$ to keep the free energy minimized. This leads directly to (58).

For the z correlations the contributing eigenvalue is $\mathrm{d}\lambda_1^0$ and a calculation similar to the above gives the results

$$(K_1^0)^2 = 1/2\mu + \mathrm{O}(1/\mu^2) \tag{59}$$

$$\langle z_j z_{j+r} \rangle = \left[\frac{\mathrm{i}\,\mathrm{dn}\,\alpha}{1+\mathrm{sn}\,\alpha} + \mathrm{O}\left(\frac{1}{\mu}\right)\right]^r \left[\frac{1}{2\mu} + \mathrm{O}\left(\frac{1}{\mu^2}\right)\right] \tag{60}$$

$$\chi_z \sim \frac{1}{2(a-c)}. \tag{61}$$

Since the low temperature results above have been derived by means of asymptotic expansions we are not able to choose parameters freely to examine limiting cases. It is clear from the working that we are barred, for example, from taking $k = 0$ or from proceeding to the isotropic case. We may without difficulty take the limit corresponding to $b = c = 0$, as we did in I, but although our results then agree with those of Thompson (1968) to leading order the comparison is not really meaningful in the absence of the correction terms. A calculation of these higher terms would be of interest but, as the requisite mathematical results do not yet exist, would at present be prohibitively complicated.

References

Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)
Arscott F M 1964 *Periodic Differential Equations* (Oxford: Pergamon)
Arscott F M and Sleeman B D 1970 *Mathematika* **17** 39–46
Byrd P F and Friedman M D 1971 *Handbook of Elliptic Integrals* (Berlin: Springer-Verlag)
Gradshteyn I S and Ryzhik I M 1965 *Table of Integrals, Series and Products* (New York: Academic Press)
Joyce G S 1967 *Phys. Rev. Lett.* **19** 581–3
Langer R E 1934 *Trans. Am. Math. Soc.* **36** 90–106
Malurkar S L 1935 *Ind. J. Phys.* **9** 45–80
Müller H J W 1966a *Math. Nachr.* **31** 89–101
—— 1966b *Math. Nachr.* **32** 49–62 157–72
Rae J 1974 *J. Phys.* A: *Math., Nucl. Gen.* **7** 1349–59
—— 1975 *J. Phys.* A: *Math. Gen.* **8** 357–68
Thompson C J 1968 *J. Math. Phys.* **9** 241–5
Whittaker E T and Watson G N 1965 *Modern Analysis* (Cambridge: University Press) chap 16