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Distribution of zeros of the partition function of the antiferromagnetic Husimi–Temperley model II

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Abstract. This paper is concerned with determining the distribution of zeros of the partition function in the antiferromagnetic case. A principle to determine the limiting locus of zeros of the partition function in the complex fugacity plane has been proposed in a previous paper with a plausible argument and the locus was obtained for the antiferromagnetic Husimi–Temperley model. The principle states that the locus is obtained as the place where the real parts of two branches of $\chi(z)$ (\equiv analytic continuation of $\lim 1/N \ln Z$, where Z is the partition function), whose real parts are the largest and the next largest among several branches, take the same value. Now the proof of the principle is given for the AHT model. The principle is intuitively plausible and it is suggested that it may work for quite a wide class of models.

1. Introduction

This paper is concerned with determining the distribution of zeros of the partition function in the antiferromagnetic case. In a previous paper (Ohminami *et al* 1972, to be referred to as OAK) an exactly soluble model for the antiferromagnet (antiferromagnetic Husimi–Temperley (AHT) model) was introduced and the distribution of zeros of the partition function in the fugacity plane for the model was obtained. The model is defined in such a way that a lattice can be divided into two equivalent sublattices and all pair interaction energies between spins on the same sublattice are $-\gamma J\sigma_i\sigma_j/N$, and those on the opposite sublattice are $-J\sigma_i\sigma_j/N$ ($J < 0$ for the antiferromagnetic interaction).

In OAK the locus of zeros was obtained as the place where the real parts of the two branches of the complex free energies, whose real parts are the smallest and the next smallest (real parts of $\ln Z$ the largest and the next largest) among several branches, take the same value. This description was given in OAK with a plausible argument in the analogy to the case where the transfer matrix method is applicable (Katsura and Ohminami 1972, Ohminami *et al* 1972, § 3). For a one-dimensional hard core gas the principle of the maximum of $\text{Re} \ln Z$ has been proved by Penrose and Elvey (1968). In this paper the proof of the principle is given for the AHT model. The principle seems to work for a wide class of models.

2. Asymptotic form of the partition function

The partition function of the antiferromagnetic Husimi–Temperley model is written as

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$$Z(T, H, N) = \sum_{n_x=0}^{N/2} \sum_{n_\beta=0}^{N/2} \binom{N/2}{n_x} \binom{N/2}{n_\beta} \exp\left(-\frac{mH}{kT}(2n_x + 2n_\beta - N) - \frac{\gamma J}{2kT}\right) \times \exp\left\{\frac{J}{2NkT}\left(\frac{1+\gamma}{2}(N-2n_x-2n_\beta)^2 - \frac{1-\gamma}{2}(2n_x-2n_\beta)^2\right)\right\}. \quad (2.1)$$

For the explanation of the model and notation, see OAK. Equation (2.1) is transformed into

$$Z(T, H, N) = \frac{1}{\pi} \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dv e^{-\gamma J/2kT} \exp\left[\left\{\frac{mH}{kT} - 2\left(\frac{J}{2NkT} \frac{1+\gamma}{2}\right)^{1/2} u\right\} N\right] \times \exp(-u^2 - v^2) \sum_{n_x=0}^{N/2} \binom{N/2}{n_x} \exp\left[\left\{-\frac{2mH}{kT} + 4\left(\frac{J}{2NkT} \frac{1+\gamma}{2}\right)^{1/2} u + 4\left(\frac{-J}{2NkT} \frac{1-\gamma}{2}\right)^{1/2} v\right\} n_x\right] \sum_{n_\beta=0}^{N/2} \binom{N/2}{n_\beta} \exp\left[\left\{-\frac{2mH}{kT} + 4\left(\frac{J}{2NkT} \frac{1+\gamma}{2}\right)^{1/2} u - 4\left(\frac{-J}{2NkT} \frac{1-\gamma}{2}\right)^{1/2} v\right\} n_\beta\right]. \quad (2.2)$$

Here we used the transformation

$$e^{s^2} = \pi^{-1/2} \int_{-\infty}^{\infty} \exp(-u^2 + 2su) du \quad (2.3a)$$

$$e^{-s^2} = \pi^{-1/2} \int_{-\infty}^{\infty} \exp(-v^2 - 2isv) dv. \quad (2.3b)$$

for real s . The summation in equation (2.2) can be carried out and gives

$$Z(t, h, N) = \frac{-NJ}{8kT} e^{-\gamma J/2kT} \frac{1}{\pi} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy e^{Nf(x,y)}, \quad (2.4)$$

where

$$f(x, y) = -\frac{1}{4t}(x^2 + y^2) + \frac{1}{2} \ln \left(2 \cosh \frac{h - i\{(1+\gamma)/2\}^{1/2}x + \{(1-\gamma)/2\}^{1/2}y}{t} \right) + \frac{1}{2} \ln \left(2 \cosh \frac{h - i\{(1+\gamma)/2\}^{1/2}x - \{(1-\gamma)/2\}^{1/2}y}{t} \right) \quad (2.5)$$

and

$$h = \frac{2mH}{-J}, \quad t = \frac{2kT}{-J} \quad (2.6)$$

$$\frac{x}{t} = \left(\frac{-2J}{NkT}\right)^{1/2} u, \quad \frac{y}{t} = \left(\frac{-2J}{NkT}\right)^{1/2} v.$$

When the real temperature t and the complex magnetic field h are given, points x, y which maximize $\text{Re } f(x, y)$ are obtained from

$$\frac{\partial f}{\partial x} = 0, \quad \frac{\partial f}{\partial y} = 0 \quad (2.7)$$

hence they are given by coupled equations

$$x = -i \left(\frac{1+\gamma}{2} \right)^{1/2} \left(\tanh \frac{h - i\{(1+\gamma)/2\}^{1/2}x + \{(1-\gamma)/2\}^{1/2}y}{t} + \tanh \frac{h - i\{(1+\gamma)/2\}^{1/2}x - \{(1-\gamma)/2\}^{1/2}y}{t} \right) \tag{2.8a}$$

and

$$y = \left(\frac{1-\gamma}{2} \right)^{1/2} \left(\tanh \frac{h - i\{(1+\gamma)/2\}^{1/2}x + \{(1-\gamma)/2\}^{1/2}y}{t} - \tanh \frac{h - i\{(1+\gamma)/2\}^{1/2}x - \{(1-\gamma)/2\}^{1/2}y}{t} \right). \tag{2.8b}$$

The coupled equations (2.8a) and (2.8b) can be decomposed into two equations each of which contains only x, h, t and only y, h, t (see equations (4.6) and (4.9)).

In general we have an infinite number of pairs x, y , which satisfy (2.8a) and (2.8b) for given t and h or t and the fugacity $z (\equiv e^{-2h/t})$. They are different branches of an analytic function defined by equations (2.8a) and (2.8b). The function $f(x, y)$ regarded as a function of z is a many-valued function and is denoted by $\chi(z) (\equiv f(x(z), y(z)))$. First we consider the case where there exists only one pair x, y which makes $\text{Re } f(x, y)$ the largest among branches of $f(x, y)$. Let the point be denoted by x_0, y_0 , and the function $f(x_0, y_0)$ regarded as a one-valued function of z by $\chi_{\max}(z) (\equiv f(x_0(z), y_0(z)))$. Expanding $f(x, y)$ at x_0, y_0 , and evaluating the integral by the contribution of the integrand near x_0, y_0 , we have (see Appendix)

$$\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dx e^{Nf(x,y)} = \frac{2\pi}{N|f_{xx}f_{yy} - f_{xy}^2|^{1/2}} \exp(Nf(x_0, y_0)) \tag{2.9}$$

$$\sim \exp\{N(\text{Re } f(x_0, y_0) + i \text{Im } f(x_0, y_0))\}. \tag{2.9'}$$

In the limit $N \rightarrow \infty$ we have

$$\lim_{N \rightarrow \infty} (Z(t, z, N))^{1/N} = \exp(f(x_0, y_0)). \tag{2.10}$$

Suppose z moves along a curve in the complex z plane. When z gets to a point at which the largest and the second largest among $\text{Re } f(x_i, y_i)$ become equal (the branches are denoted by $f(x_1, y_1)$ and $f(x_2, y_2)$) and at which $\text{Im } f(x_1, y_1) \neq \text{Im } f(x_2, y_2)$, the contributions of these two saddle points become of the same order, and hence for such z , we have

$$Z(t, z, N) \sim \exp(N \text{Re } f(x_1, y_1)) \{ \exp(iN \text{Im } f(x_1, y_1)) + \exp(iN \text{Im } f(x_2, y_2)) \}. \tag{2.11}$$

A set of points at which the largest and the second largest of $\text{Re } f(x, y)$ are equal, makes an arc in the complex z plane. In a region which does not contain such arcs, $\chi_{\max}(z)$ is regular. On such arcs $\chi_{\max}(z)$ is discontinuous though $\text{Re } \chi(z)$ can be continuous (phase transitions in the complex h or complex z plane). Phase transition of the ferromagnet in real z was clarified using such a mechanism by Husimi (1953, see also Katsura 1955). The present paper is an application of the principle to the antiferromagnets in the complex z plane.

3. Zeros of the partition function

In this section we will give a prescription for obtaining the zeros of the partition function with its proof. First we prove a theorem.

Theorem. Define

$$\chi_N(z) \equiv \frac{1}{N} \ln Z(t, z, N). \quad (3.1)$$

Let R be a region in the complex z plane in which zeros of $Z(t, z, N)$ do not exist for $N > N_0$. Then $\chi_{\max}(z)$ is regular in R .

Proof. $\chi_N(z)$ has no poles and singularities except zeros of $Z_N(t, z, N)$. In any closed region D in R we can take M independent of N and z such that $|\chi_N(z)| < M$. From (2.10), $\chi_N(z)$ tends to $\chi_{\max}(z)$ in R . Hence by Vitali's theorem $\chi_{\max}(z)$ is regular in D . Since we can take any closed region as D in R , $\chi_{\max}(z)$ is regular in R and hence the theorem is proved.

The theorem is an extension† of the theorem of Yang and Lee (1952, theorem 2, see also Huang 1963). Hence by the contraposition of the theorem, a point at which $\chi_{\max}(z)$ is not regular, is a limit point of zeros of the partition function. Thus an arc on which $\chi_{\max}(z)$ is not regular, obtained as a point where $\text{Re } f(x_1, y_1) = \text{Re } f(x_2, y_2)$ and $\text{Im } f(x_1, y_1) \neq \text{Im } f(x_2, y_2)$, is a set of limit points of zeros of the partition function.

Indeed comparison of (2.9) and (2.11) shows that we cannot make $|Z(t, z, N)| < \epsilon$ in a given neighbourhood of z at which only one $\chi_{\max}(z)$ exists, while $Z(t, z, N) = 0$ is possible only in the neighbourhood of z at which $\text{Re } f(x_1, y_1) = \text{Re } f(x_2, y_2)$. It is to be noted that the reverse of the Yang–Lee theorem does not hold for the antiferromagnetic case (while it does for the ferromagnetic case). When we take a region R inside which $\chi_{\max}(z)$ is regular, then zeros of $Z(t, z, N)$ cannot be generally excluded for such a region even for sufficiently large N . (When we take a point z_0 and a neighbourhood of z_0 in R , zeros of $Z(t, z, N)$ can be excluded for sufficiently large N in this neighbourhood.)

Thus the prescription for obtaining the locus of zeros of the partition function was proved as a necessary and sufficient condition. The loci of zeros obtained by this prescription have already been shown in OAK. The circle theorem for the ferromagnetic Husimi–Temperley model can also be proved by the present method, though it is a direct consequence of the Lee–Yang theorem for the Ising ferromagnet (Katsura 1955).

4. Reduction of coupled equations (2.8a) and (2.8b)

The magnetization σ (per spin) is given by

$$\begin{aligned} \sigma = t \frac{\partial \ln Z/N}{\partial h} &= \frac{\partial f}{\partial h} + \frac{\partial f}{\partial x} \frac{\partial x}{\partial h} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial h} = \frac{1}{2} \tanh \frac{h - i\{(1+\gamma)/2\}^{1/2}x + \{(1-\gamma)/2\}^{1/2}y}{t} \\ &+ \frac{1}{2} \tanh \frac{h - i\{(1+\gamma)/2\}^{1/2}x - \{(1-\gamma)/2\}^{1/2}y}{t}. \end{aligned} \quad (4.1)$$

†. Modifications of the Yang–Lee theorem presented here (R may not include the real axis, and add *for $N > N_0$) are irrelevant to the essentiality of the Yang–Lee theorem.

When we put

$$\begin{aligned}x &= -i \left(\frac{1+\gamma}{2} \right)^{1/2} (\sigma_\alpha + \sigma_\beta) \\y &= \left(\frac{1-\gamma}{2} \right)^{1/2} (\sigma_\alpha - \sigma_\beta)\end{aligned}\tag{4.2}$$

equations (2.8a) and (2.8b) are transformed into

$$\begin{aligned}\sigma_\alpha &= \tanh \frac{h - \sigma_\beta - \gamma \sigma_\alpha}{t} \\ \sigma_\beta &= \tanh \frac{h - \sigma_\alpha - \gamma \sigma_\beta}{t}\end{aligned}\tag{4.3}$$

and we see that σ_α and σ_β are the complex magnetization of sublattices α and β . In terms of σ_α and σ_β , the negative of the complex (Helmholtz) free energy multiplied by t (equation (2.5)) is written in

$$\begin{aligned}f(x, y) &= \frac{1}{4t} \{2\sigma_\alpha \sigma_\beta + \gamma(\sigma_\alpha^2 + \sigma_\beta^2)\} + \frac{1}{2} \ln \left(2 \cosh \frac{h - \sigma_\beta - \gamma \sigma_\alpha}{t} \right) \\ &\quad + \frac{1}{2} \ln \left(2 \cosh \frac{h - \sigma_\alpha - \gamma \sigma_\beta}{t} \right).\end{aligned}\tag{4.4}$$

Eliminating h , we have

$$f(x, y) = \frac{1}{4t} \{2\sigma_\alpha \sigma_\beta + \gamma(\sigma_\alpha^2 + \sigma_\beta^2)\} - \frac{1}{4} \ln(1 - \sigma_\alpha^2) - \frac{1}{4} \ln(1 - \sigma_\beta^2) + \ln 2.\tag{4.5}$$

In terms of $\sigma_\alpha + \sigma_\beta$ and $\sigma_\alpha - \sigma_\beta$ the coupled equations (2.8a) and (2.8b) to determine x and y are decomposed into two independent equations

$$\sigma_\alpha + \sigma_\beta = \frac{tS_1 \operatorname{arccosh} A}{(1-\gamma)(A^2-1)^{1/2}}\tag{4.6}$$

$$A = \frac{2S_1}{\sigma_\alpha + \sigma_\beta} - C_1\tag{4.7}$$

$$S_1 = \sinh \frac{2h - (1+\gamma)(\sigma_\alpha + \sigma_\beta)}{t}\tag{4.8}$$

$$C_1 = \cosh \frac{2h - (1+\gamma)(\sigma_\alpha + \sigma_\beta)}{t}$$

and

$$\sigma_\alpha - \sigma_\beta = \frac{S_2(2h - t \operatorname{arccosh} B)}{(1+\gamma)(B^2-1)^{1/2}}\tag{4.9}$$

$$B = \frac{2S_2}{\sigma_\alpha - \sigma_\beta} - C_2\tag{4.10}$$

$$S_2 = \sinh \frac{(1-\gamma)(\sigma_\alpha - \sigma_\beta)}{t}$$

$$C_2 = \cosh \frac{(1-\gamma)(\sigma_\alpha - \sigma_\beta)}{t}.$$
(4.11)

Equation (4.6) with equations (4.7) and (4.8) contains only $\sigma_\alpha + \sigma_\beta$, and equation (4.9) with equations (4.10) and (4.11) contains only $\sigma_\alpha - \sigma_\beta$.

We consider the case for real h . Equation (4.9) always has a solution in which $\alpha_x = \sigma_\beta$ ($y = 0$). It has two real solutions $\sigma_\alpha - \sigma_\beta = \pm \{(1-\gamma)/2\}^{-1/2} y_1$ at low temperature and at low field. These two solutions become pure imaginary at high temperature. The solution $y = 0$ is a paramagnetic state. Equation (4.6) was derived under the condition $\sigma_\alpha \neq \sigma_\beta$. When $\sigma_\alpha = \sigma_\beta$, equation (4.6) is replaced by

$$\sigma_p = \tanh \frac{h - (1+\gamma)\sigma_p}{t}$$
(4.12)

where $\sigma_p = (\sigma_\alpha + \sigma_\beta)/2$.

The analysis of the solutions (4.6) and (4.9) clarifies that the antiferromagnetic free energy is lower than the paramagnetic free energy in the antiferromagnetic state (see Appendix).

5. Conclusion

This paper is concerned with determining the distribution of zeros of the partition function in the antiferromagnetic case. A principle was proposed and used in obtaining the locus of the AHT model in a previous paper. The principle states that the locus is obtained as the point where the real parts of two branches of $\chi(z)$, whose real parts are the largest and the next largest, take the same value. In that paper a plausible argument was used by analogy with the case where the transfer matrix method is applicable (Katsura and Ohminami 1972, Ohminami *et al* 1972, § 3).

In this paper the proof of the principle was given for the case of the AHT model. The principle is now proved to work for the one-dimensional hard rod model (Penrose and Elvey 1968), the one-dimensional antiferromagnetic model (Katsura and Ohminami 1972), and the ferromagnetic and antiferromagnetic Husimi–Temperley models. The principle seems to work for a wide class of models. Ever since the work of Yang and Lee (1952) there has been a need for a similar theorem in the antiferromagnetic type of case. The suggested principle, if provable for a wide class of cases generally, could well be one of the missing pieces of the puzzle.

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Appendix. Saddle point method for a function of two variables

Consider an integral

$$I = \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dx e^{Nf(x,y)} \tag{A.1}$$

with such a function $f(x, y)$ where $\lim_{x \rightarrow \pm \infty} \text{Re } f(x, y) = -\infty$ for fixed y and $\lim_{y \rightarrow \pm \infty} \text{Re } f(x, y) = -\infty$ for fixed x are satisfied.

First we consider $I_2 = \int_{-\infty}^{\infty} dx e^{Nf(x,y)}$ regarding y as a parameter. Let x_j be points in the complex x plane which make $\text{Re } f(x, y)$ maxima for a given y . The saddle points x_j are obtained from $\partial f / \partial x = 0$. The path of the integration is deformed to be a steepest path through the most dominant saddle point. In general x_j is a function of y . Then

$$I_2 = \sum_j \exp(Nf(x_j, y)) \int_C dx \exp\{\frac{1}{2}Nf_{xx}(x_j, y)(x - x_j)^2\} \tag{A.2}$$

where Σ_j is taken for such points x_j that lie on the steepest path C (in the complex x plane), which goes from $-\infty$ to $+\infty$ and passes through the most dominant saddle point.

We put

$$\begin{aligned} f_{xx}(x_j, y) &= R_j e^{i\Phi_j} \\ x - x_j &= r_j e^{i\phi_j} \end{aligned} \tag{A.3}$$

then the direction of the steepest line near x_j is given by

$$\phi_j = \frac{1}{2}(\pi - \Phi_j) \tag{A.4}$$

and the integration path is replaced by an infinite line with this direction at each x_j . Thus

$$\begin{aligned} I_2 &\sim \sum_j \exp(Nf_{xx}(x_j, y)) \int_{-\infty}^{\infty} e^{i\phi_j} dr_j \exp(-NR_j r_j^2/2) \\ &= \sum_j \exp(Nf(x_j, y)) \exp\{\frac{1}{2}i(\pi - \arg f_{xx}(x_j, y))\} \left(\frac{2\pi}{N|f_{xx}(x_j, y)|}\right)^{1/2}. \end{aligned} \tag{A.5}$$

Next we substitute (A.5) into (A.1)

$$I = \sum_j \int_{-\infty}^{\infty} dy \exp(Nf(x_j, y)) \exp\{\frac{1}{2}i(\pi - \arg f_{xx}(x_j, y))\} \left(\frac{2\pi}{N|f_{xx}(x_j, y)|}\right)^{1/2}. \tag{A.6}$$

Let

$$F_j(y) \equiv f(x_j(y), y) \tag{A.7}$$

and y_k the points which make $\text{Re } F_j(y)$ maxima. Replacing y by y_k except that on the exponent $Nf(x_j, y)$, and carrying out the integration in a similar way as previously,

we have

$$I = \sum_j \sum_k \exp\{i(\pi - \frac{1}{2} \arg f_{xx}(x_j, y_k))\} \left(\frac{2\pi}{N|f_{xx}(x_j, y_k)|}\right)^{1/2} \exp\{i(\pi - \frac{1}{2} \arg F_{yy}(y_k))\} \\ \times \left(\frac{2\pi}{N|F_{yy}(y_k)|}\right)^{1/2} \exp(NF(y_k)). \tag{A.8}$$

Since $x = x(y)$ is determined by $f_x(x, y) = 0$, the differentiation on F can be written as

$$\frac{dF}{dy} = \left(\frac{\partial}{\partial y} - \frac{f_{xy}}{f_{xx}} \frac{\partial}{\partial x}\right) f \tag{A.9}$$

$$\frac{d^2F}{dy^2} = \left(\frac{\partial}{\partial y} - \frac{f_{xy}}{f_{xx}} \frac{\partial}{\partial x}\right)^2 f = f_{yy} - \frac{(f_{xy})^2}{f_{xx}} - f_x \left(\frac{\partial}{\partial y} \frac{f_{xy}}{f_{xx}} - \frac{f_{xy}}{f_{xx}} \frac{\partial}{\partial x} \frac{f_{xy}}{f_{xx}}\right). \tag{A.10}$$

Hence x_j and y_k are determined by solving $f_x = 0$ and $f_y = 0$. The value of F_{yy} at y_k is given by

$$F_{yy}(y_k) = f_{yy}^{(j,k)} - (f_{xy}^{(j,k)})^2 / f_{xx}^{(j,k)} \tag{A.11}$$

where $f_{xx}^{(j,k)} = f_{xx}(x_j, y_k)$ etc.

Substituting (A.8) and (A.11) into (A.1) we have

$$I \simeq \sum_j \sum_k \exp[i\pi - \frac{1}{2}i \arg f_{xx}^{(j,k)} - \frac{1}{2}i \arg \{f_{yy}^{(j,k)} - (f_{xy}^{(j,k)})^2 / f_{xx}^{(j,k)}\}] \\ \times \frac{2\pi}{N|f_{xx}^{(j,k)} f_{yy}^{(j,k)} - (f_{xy}^{(j,k)})^2|^{1/2}} \exp(Nf(x_j, y_k)). \tag{A.12}$$

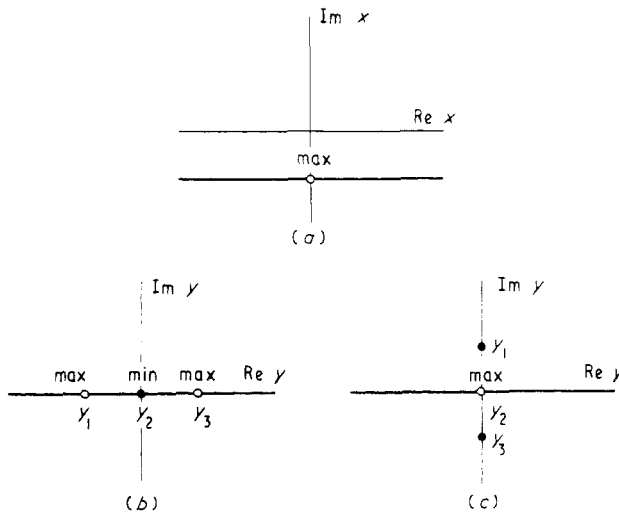


Figure 1. Saddle points and the path of the integration for real h . (a) x plane; (b) antiferromagnetic state in y plane; (c) paramagnetic state in y plane.

When N is sufficiently large, $\sum_j \sum_k$ is replaced by the largest term, which is denoted by $x_j = x_0, y_k = y_0$. Then

$$I \simeq e^{i\phi_0} \frac{2\pi}{N|f_{xx}^0 f_{yy}^0 - (f_{xy}^0)^2|^{1/2}} \exp(Nf(x_0, y_0)) \quad (\text{A.13})$$

where ϕ_0 is the value of the phase factor at (x_0, y_0) corresponding to that in (A.12).

From the analysis of § 4 we see that three important saddle points, $y_1, y_2 = 0, y_3 = -y_1$, exist in the second integral $\int_{-\infty}^{\infty} dy$. In the antiferromagnetic region, y_1 and y_3 are real, $f_{yy}(x_0, y_1) = f_{yy}(x_0, y_3) < 0, f_{yy}(x_0, y_2) > 0$ and the most dominant saddle points are y_1 and $y_3 (= y_0)$, while in the paramagnetic region, y_1 and y_3 are pure imaginary, $f_{yy}(x_0, y_1) = f_{yy}(x_0, y_3) > 0, f_{yy}(x_0, y_2) < 0$, and the most dominant saddle point is $y_2 (= y_0)$, for real h . When h goes from the antiferromagnetic region to the paramagnetic region, the most dominant saddle point changes from $y_1 (y_3)$ to y_2 at the critical field (figure 1). When h is complex, a similar situation occurs though y_1 and y_3 are neither real nor pure imaginary.

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