Direction-Dependent Free Energy Singularity of the Antiferroelectric Asymmetric Six-Vertex Model

Giuseppe Albertini[1]

The transition from the ordered commensurate phase to the incommensurate Gaussian phase of the antiferroelectric asymmetric six-vertex model is investigated by keeping the temperature constant below the roughening point and varying the external fields (h, v). In the (h, v) plane, the phase boundary is approached along straight lines $\delta v = k\,\delta h$, where $(\delta h, \delta v)$ measures the displacement from the phase boundary. It is found that the free energy singularity displays the exponent 3/2 typical of the Pokrovski–Talapov transition $\delta f \sim \text{const}(\delta h)^{3/2}$ for any direction other than the tangential one. In the latter case δf shows a discontinuity in the third derivative.

1. INTRODUCTION

The asymmetric six-vertex model is the extension of the well-known symmetric six-vertex model to the case where external fields interact with the local fluctuating variables ("dipoles" or "arrows").[1-3] On a two-dimensional square lattice, two-valued variables live on links and interact at vertices. At each vertex, of the sixteen possible configurations, only six, those with an equal number of incoming and outgoing arrows, are allowed. The relevant Boltzmann weights, which define the model, are grouped into the matrix $R_{\alpha\alpha'}^{\beta\beta'}$ as shown in Fig. 1. Throughout this paper, we choose interactions that favor antiferroelectric order, while the external homogeneous two-component field (h, v), favoring ferroelectric ordering, competes with the arrow–arrow couplings.

---

[1] Physics Department, Milan University, 20133 Milan, Italy; e-mail address: albert@osfmi. mi.infn.it.

If one treats the problem with the transfer matrix method, an exact solution is provided by the Bethe-ansatz.[1-3] The phase diagram was outlined in the original paper,[1] while further developments came more recently[2, 5-8] (the list is not exhaustive. Papers dealing with the ferroelectric regime are not included). Since the early works appeared, it has been known that, in the (h, v) plane, there is a closed curve Γ separating an antiferroelectrically ordered, commensurate region with finite correlation length, inside Γ, from an incommensurate region with infinite correlation length (critical), outside Γ. The ordered region includes the symmetric model point $(0, 0)$ and the free energy in it is field independent

$$f(\gamma, u, h, v) = f_0(\gamma, u)$$

The parameters γ, u contain the temperature dependence and will be defined in the next section. As Γ is approached from outside (i.e. from the incommensurate phase), keeping γ and u fixed, the free energy is expected to display a singularity with a characteristic exponent $3/2$. More precisely, the following result has been proven in ref. 4.

Let $(\bar{h}(b), \bar{v}(b))$ be a parametric equation of Γ, to be given later, with b some real parameter running in a bounded interval. Lieb and Wu found that, if $h = 0$, which implies $b = 0$, the singular part of the free energy is

$$f(\gamma, u, 0, \bar{v}(0) + \delta v) = f_0(\gamma, u) + \delta f(\gamma, u, \delta v) = f_0(\gamma, u) + c(\gamma, u)(\delta v)^{3/2} \quad (1)$$

yielding a divergence $\sim \delta v^{-1/2}$ for the susceptibility. (A divergence with exponent $1/2$ was also found for the specific heat at fixed field). Borrowing a terminology introduced in later years, the transition belongs to the Pokrovski–Talapov universality class.[9, 10]

Equation (1) does not clarify how the singularity depends on both field components. A further step in this direction was recently achieved by Noh and Kim[5] who extended the method of ref. 11 to relate macroscopic quantities such as susceptivities to finite size corrections of transfer matrix spectra. They showed that, in the critical phase

$$\begin{vmatrix} \dfrac{\partial^2 f}{\partial h^2} & \dfrac{\partial^2 f}{\partial h \, \partial v} \\ \dfrac{\partial^2 f}{\partial v \, \partial h} & \dfrac{\partial^2 f}{\partial v^2} \end{vmatrix} = \left(\dfrac{2}{\pi g} \right)^2 \quad (2)$$

where g is the coupling constant of the gaussian model on which the critical incommensurate phase renormalizes. As Γ is approached from this phase, $g \to 2$.

In this paper, the question is settled of how, at fixed y, u the singularity of $f(h, v)$ depends on both (h, v). The underlying motivation is that the solvability of the model for arbitrary (h, v) provides a way to study exactly how the leading singular part of the free energy depends on more than one parameter near the phase transition. Does the singular behavior depends on how the transition line is approached? While finding the leading singularity as a function of (h, v) simultaneously has proven to be elusive, it will be shown that the singularity does depend on the direction in the (h, v) plane.

The results are best summarized if one introduces the following notation. Set

$$v_t(b) = \frac{d}{db} \bar{v}(b) \qquad h_t(b) = \frac{d}{db} \bar{h}(b)$$

$$v_1(b) = \frac{d}{db} v_t(b) \qquad h_1(b) = \frac{d}{db} v_t(b)$$

$$\Delta = v_t h_1 - h_t v_1$$

Next, consider a variation into the incommensurate phase $h = \bar{h}(b) + \delta h$, $v = \bar{v}(b) + \delta v$ where $\delta v = k \, \delta h$ and k fixes a slope not tangential to Γ. Then

$$\delta f(\delta h) = \left(\frac{h_t}{\Delta}\right)^{1/2} \frac{h_t}{3\pi} \left[2 \left(k - \frac{v_t}{h_t}\right) \delta h \right]^{3/2} \tag{3}$$

so the singularity is governed by an exponent $3/2$ for all these directions. Yet, if Γ is approached tangentially, which amounts to take $\delta v = [v_t/h_t] \, \delta h$

$$\delta f(\delta h) = \begin{cases} c_+ \delta h^3 & \text{if} \quad \delta h > 0 \\ c_- \delta h^3 & \text{if} \quad \delta h < 0 \end{cases} \tag{4}$$

where $c_+ \neq c_-$ are b-dependent and are given in Eq. (38). In other words there is a jump in the third derivative. The calculation breaks down at the two points on Γ where $h_t = 0$, i.e. where the tangent to Γ is parallel to the v-axis. Those cases were examined in ref. 8 and an analogous conclusion was reached.

Besides being a sensible statistical model in itself, the asymmetric six-vertex model has been mapped many times on various kinds of SOS models[15, 16] which, in turn, are often used as simple models of crystals at equilibrium. Then, the free energy as function of (h, v) describes the surface of the crystal and the phase of constant free energy corresponds to a flat crystal facet whose boundary is Γ. The results of this paper provide a fine description of how the crystal surface bends near the facet edge.

The paper is divided as follows. Section 2 presents a summary of the Bethe ansatz and already known results. Section 3 deals with a perturbative expansion of the integral equations typical of the Bethe ansatz and Section 4 exploits that expansion to determine the singularities of the free energy.

2. BASIC DEFINITIONS AND SUMMARY OF BETHE ANSATZ

The Boltzmann weights, as given in Fig. 1, are functions of the spectral parameter u, a notation that seems more natural in the framework of the Bethe ansatz. Row-to-row transfer matrices

$$T(u)_{\alpha, \alpha'} = \sum_{\underline{\beta}} \prod_{k=1}^{N} R_{\alpha_k \alpha_k'}^{\beta_k \beta_{k+1}}(u)$$

with periodic boundary conditions $(\beta_{N+1} = \beta_1)$ commute for different values of the spectral parameter

$$[T(u), T(u')] = 0$$

Arrow conservation at each vertex, and periodic boundary conditions, imply that $T(u)$ breaks into blocks between states with the same number of up (and down) arrows. Let n be the number of arrows reversed with respect to the reference state $| \uparrow \uparrow, ..., \uparrow \rangle$. The Bethe ansatz provides the following solution to the eigenvalue problem for $T(u)$:[1-3, 8]

$$A(u) = e^{v(N-2n)+hN} \left[\frac{\sinh(\gamma - u)}{\sinh \gamma} \right]^N \prod_{j=1}^{n} \frac{\sinh((\gamma/2) + u - (i\alpha_j/2))}{\sinh((\gamma/2) - u + (i\alpha_j/2))}$$

$$+ e^{v(N-2n)-hN} \left[\frac{\sinh u}{\sinh \gamma} \right]^N \prod_{j=1}^{n} \frac{\sinh(-(3\gamma/2) + u - (i\alpha_j/2))}{\sinh((\gamma/2) - u + (i\alpha_j/2))} \tag{5}$$

is an eigenvalue if the "rapidities" $\{\alpha_j\}$, $j = 1, 2, ..., n$ satisfy the set of equations

$$\left[\frac{\sinh((\gamma/2) + (i\alpha_j/2))}{\sinh((\gamma/2) - (i\alpha_j/2))} \right]^N$$

$$= (-)^{n+1} e^{2hN} \prod_{k=1}^{n} \frac{\sinh(\gamma + (i/2)(\alpha_j - \alpha_k))}{\sinh(\gamma - (i/2)(\alpha_j - \alpha_k))} \qquad j = 1, 2, ..., n \tag{6}$$

In the limit $N \to \infty$, the rapidities $\{\alpha_j\}$ condense into curves in the complex plane, and are conveniently described by a density function $R(\alpha)$

$$R(\alpha_j) = \lim_{N \to \infty} \frac{2\pi}{N(\alpha_{j+1} - \alpha_j)}$$

Eqs. (6) are replaced by a single linear integral equation that governs the thermodynamics of the model. Introduce the functions (this notation is somewhat redundant, but it has been adopted in many previous papers and it will be kept here)

$$p^0(\alpha) = -i \log \left[\frac{\sinh((\gamma/2) + (i\alpha/2))}{\sinh((\gamma/2) - (i\alpha/2))} \right]$$

$$\Theta(\alpha) = -i \log \left[\frac{\sinh(\gamma + (i\alpha/2))}{\sinh(\gamma - (i\alpha/2))} \right]$$

$$\xi(\alpha) = \frac{dp^0(\alpha)}{d\alpha}$$

$$K(\alpha) = \frac{d\Theta(\alpha)}{d\alpha}$$

and the vertical polarization

$$y = \lim_{N \to \infty} \left(1 - \frac{2n}{N} \right) \tag{7}$$

Then, for a state described by a rapidity curve C, the density $R(\alpha)$ solves[1, 2, 8]

$$\xi(\alpha) - \frac{1}{2\pi} \int_C d\beta \, K(\alpha - \beta) \, R(\beta) = R(\alpha) \tag{8}$$

and

$$p^0(\alpha) - \frac{1}{2\pi} \int_C d\beta \, \Theta(\alpha - \beta) \, R(\beta) + 2ih = 2\pi x \qquad -\frac{1-y}{4} \leqslant x \leqslant \frac{1-y}{4} \tag{9}$$

where x is the real parameter of the curve. Let $A = -a + ib$, $B = a + ib$ be the two endpoints of the curve. (We take for granted that $B = -A^*$ because we wish to consider, in each sector of fixed n, the largest transfer matrix eigenvalue, which is real and unique by Perron–Froboenius

theorem.[13] Since $\{\alpha_j\} \to \{-\alpha_j^*\}$ is a symmetry of (6) we expect it to hold for the solution corresponding to the unique largest eigenvalue in each sector). Solution of (8) implicitly depends on the endpoints A, B and contributes to make y, h dependent on a, b through[1,2,8]

$$\frac{1-y}{2} = \frac{1}{2\pi} \int_A^B d\alpha \, R(\alpha; A, B) \tag{10}$$

$$p^0(A) + p^0(B) - \frac{1}{2\pi} \int_A^B d\beta \, R(\beta; A, B)[\Theta(A-\beta) + \Theta(B-\beta)] + 4ih = 0 \tag{11}$$

In the transfer matrix formalism, the free energy is determined by the largest eigenvalue Λ_0, so, neglecting a factor $1/k_B T$

$$f(u, \gamma, h, v) = -\lim_{N \to \infty} \frac{\ln \Lambda_{N,0}(u, \gamma, h, v)}{N} \tag{12}$$

With an abuse of language, the relevant eigenstate will be called "ground state." From (5), all eigenvalues are such that $\Lambda(u) = \Lambda_R(u) + \Lambda_L(u)$. One of the two addends dominates over the others for specific values of the parameters. We set

$$\lim_{N \to \infty} \frac{1}{N} \ln \Lambda_R(u)$$

$$= F_R(u, \gamma, h, y) + vy$$

$$= h + \ln \frac{\sinh(\gamma - u)}{\sinh \gamma} + \frac{1}{2\pi} \int_A^B d\alpha \, R(\alpha; A, B) \, f_R(\alpha, u) \tag{13}$$

$$\lim_{N \to \infty} \frac{1}{N} \ln \Lambda_L(u)$$

$$= F_L(u, \gamma, h, y) + vy$$

$$= -h + \ln \frac{\sinh u}{\sinh \gamma} + \frac{1}{2\pi} \int_A^B d\alpha \, R(\alpha; A, B) \, f_L(\alpha; u) \tag{14}$$

with

$$f_R(\alpha; u) = \ln \frac{\sinh((\gamma/2) + u - (i\alpha/2))}{\sinh((\gamma/2) - u + (i\alpha/2))}$$

$$f_L(\alpha; u) = \ln \frac{\sinh(-(3\gamma/2) + u - (i\alpha/2))}{\sinh((\gamma/2) - u + (i\alpha/2))}$$

and call $F = \max\{F_R, F_L\}$. The equilibrium polarization and the free energy are then determined by

$$f(u, \gamma, h, v) = \min_{-1 \leqslant y \leqslant 1} (-F(u, \gamma, h, y) - vy) = \min_{-1 \leqslant y \leqslant 1} \mathscr{F}(u, \gamma, h, v, y) \quad (15)$$

The ground state solution of (8) is explicitly computed when h and v are sufficiently small.[1-3, 8] It corresponds to $n = N/2$ and, in the $N \to \infty$ limit, to $a = \pi$, $-\gamma \leqslant b \leqslant \gamma$. Then (8) can be solved by Fourier transform. Even though the solution has appeared many times in the literature, it is worthwhile to recall it here to introduce the elliptic function notation

$$R(\alpha; -\pi + ib, \pi + ib) = \sum_{n=-\infty}^{+\infty} \frac{e^{-in\alpha}}{2\cosh(n\gamma)} = \frac{I(k)}{\pi} \, dn\left(\frac{I(k)\alpha}{\pi}; k\right) \quad (16)$$

where $I'(k)/I(k) = \gamma/\pi$ and $I(k)(I'(k))$ is the complete elliptic integral of the first kind with modulus $k(k' = \sqrt{1-k^2})$. Replacing (16) into (10) and (11) yields[1-3, 8]

$$y = 0 \qquad \bar{h}(b) = Z(-b) \quad (17)$$

where

$$Z(x) \overset{\text{def}}{=} \frac{x}{2} + \sum_{n=1}^{\infty} \frac{(-)^n}{n} \frac{\sinh(nx)}{\cosh(n\gamma)} \quad (18)$$

Within the range $-\gamma \leqslant b \leqslant \gamma$ there is a crossing between Λ_R and Λ_L. Let's call id the point where the ground state curve meets the imaginary axis in the α-plane. It turns out that Λ_R dominates when $d < \gamma - 2u$ while Λ_L does when $d > \gamma - 2u$. One can check it by replacing (16) into (13), (14), or, more quickly, by the following argument. Select chains such that $n = N/2$ is an odd number. By virtue of the symmetry $\{\alpha_j\} \to \{-\alpha_j^*\}$ one α, say $\bar{\alpha}$, has to be pure imaginary. The other $n - 1$ $\{\alpha_j\}$ can be paired to give a positive contribution to Λ_R and Λ_L so the contribution of $\bar{\alpha}$ determines the sign of Λ_R and Λ_L. It is easily seen that

$$\Lambda_R(\bar{\alpha}) > (<) 0 \qquad \text{if} \quad \text{Im } \bar{\alpha} < (>) \gamma - 2u$$

$$\Lambda_L(\bar{\alpha}) > (<) 0 \qquad \text{if} \quad \text{Im } \bar{\alpha} > (<) \gamma - 2u$$

In the thermodynamic limit $\text{Im } \alpha \to d$, and since by Perron-Froboenius theorem $\Lambda_{N, \max}$ must be positive, we get the desired result. When crossing,

$$e^{h+v}\,\frac{\sinh(\gamma-u)}{\sinh\gamma} = e^{\beta(\delta/2-\epsilon)+h+v} = R^{11}_{11}(u)$$

$$e^{-h-v}\,\frac{\sinh(\gamma-u)}{\sinh\gamma} = e^{\beta(\delta/2-\epsilon)-h-v} = R^{22}_{22}(u)$$

$$e^{-h+v}\,\frac{\sinh u}{\sinh\gamma} = e^{\beta(-\delta/2-\epsilon)-h+v} = R^{22}_{11}(u)$$

$$e^{h-v}\,\frac{\sinh u}{\sinh\gamma} = e^{\beta(-\delta/2-\epsilon)+h-v} = R^{11}_{22}(u)$$

$$1 = 1 = R^{12}_{21}(u)$$

$$1 = 1 = R^{21}_{12}(u)$$

Fig. 1. Boltzmann weights in the notation with spectral parameter u compared to that of ref. 2. The physical region is $0 < u < \gamma$.

though, Λ_R and Λ_L connect smoothly, so no singularity of f appears and one finds from (13), (14) the field independent value of the symmetric six-vertex model[12]

$$f(u, \gamma, h, v) = -2 \sum_{n=1}^{+\infty} \frac{e^{-2\gamma n}}{n \cosh(\gamma n)} \sinh(nu)\sinh(\gamma - u) \qquad 0 \leqslant u \leqslant \gamma \qquad (19)$$

The region in the (h, v) plane where (19) is valid is bounded by (17) and the value of the v-field at which the ground state moves away from the $y = 0$ sector. This is fixed by the equation

$$\bar{v}(b) = -\frac{\partial F}{\partial y}\bigg|_{h\,\text{fixed},\,y\,=\,0} \qquad (20)$$

that yields[1–3, 8]

$$\bar{v}(b) = Z(\gamma - |\gamma - 2u - b|) \qquad -\gamma \leqslant b \leqslant \gamma \tag{21}$$

More precisely, $\bar{v}(b)$ in (21) runs over half of the curve, the other half is obtained from the symmetry $f(h, v) = f(-h, -v)$, which follows trivially from reversal of all arrows in the statistical sum. Eqs. (17) and (21) provide the parametric equation $(\bar{h}(b), \bar{v}(b))$ of Γ.

Equation (19) is the free energy of the symmetric six-vertex model in the ordered antiferroelectric phase. As the temperature is increased, the model undergoes a phase transition at $\gamma = 0$ where the free energy in non-analytic but continuous with all its derivatives.[12] If the six-vertex model is mapped into a BCSOS model,[15, 2] the transition corresponds to the roughening point. Therefore, when working with the Boltzmann weights defined in Fig. 1, one is at temperatures below the roughening point T_R. It can be checked that, at T_R, the curve defined by (17) and (21) shrinks to a point.[2]

3. THE EXPANSION IN δa, δb

Equations (8), (10), (11), (13), (14) determine the thermodynamics of the system. In principle, one should solve (8) and plug $R(\alpha; A, B)$ into the others. This would give

$$y = y(a, b) \qquad h = h(a, b) \qquad F = F(a, b)$$

Once the first two are inverted and plugged into the third, one can minimize $-F(\gamma, v, h, y) - vy$ w.r. to y keeping h, v fixed. Of course, (8) is not exactly solvable for $a \neq \pi$. Therefore we attempt an expansion that generalizes the method that Lieb and Wu[4] applied to the $h = 0$ case, where the rapidities are real $(b = 0)$ and everything is a function of a only. Namely, it will be assumed that a unique solution exists for (8) at least in a narrow neighborhood of the segment $a = \pi$, $-\gamma < b < \gamma$ and that the dependence of $R(\alpha; A, B), y(A, B), h(A, B), F(A, B)$ is analytical on A and B in this neighborhood. This assumption is partly warranted by the fact that, if a solution exists for (8), it develops a pole at $\alpha = \pm i\gamma$, where $\zeta(\alpha)$ has poles. In the following calculation, the endpoints are kept far away from the singularities of the inhomogeneous term. With this assumption, variations can be computed by taking derivatives in the relevant integral equations. One starts with (8)

$$\partial_A R(\alpha; A, B) + \frac{1}{2\pi} \int_A^B d\beta \, K(\alpha - \beta) \, \partial_A R(\beta; A, B)$$

$$= \frac{1}{2\pi} K(\alpha - A) \, R(A; A, B) \qquad (22)$$

$$\partial_B R(\alpha; A, B) + \frac{1}{2\pi} \int_A^B d\beta \, K(\alpha - \beta) \, \partial_B R(\beta; A, B)$$

$$= -\frac{1}{2\pi} K(\alpha - A) \, R(B; A, B) \qquad (23)$$

and so forth by taking further derivatives. When $A = A_0 = -\pi + ib$ and $B = B_0 = \pi + ib$, $-\gamma < b < \gamma$ all these equations can be solved by Fourier transform. For instance

$$\partial_A R(\alpha; A_0, B_0) = \frac{c_1}{2\pi} \sum_{n=-\infty}^{+\infty} e^{-in\alpha}(-)^n \frac{e^{-nb-\gamma|n|}}{2\cosh n\gamma} = -\partial_B R(\alpha; A_0, B_0)$$

$$c_1 = R(A_0; A_0, B_0) = R(B_0; A_0, B_0)$$

Notice that $c_1 = 0$ if $b = \pm\gamma$. This case was dealt with in ref. 8. The solution is replaced into the analogous expansion for $y(A, B)$, $h(A, B)$ and $F_R(A, B)$ (we will consider only the domain where $F_R > F_L$, that is $d < \gamma - 2u$). As an example, at the first order

$$\frac{\partial y}{\partial A} = -\frac{2}{2\pi} \int_A^B \partial_A R(\alpha; A, B) \, d\alpha + \frac{2}{2\pi} R(A; A, B)$$

$$\frac{\partial y}{\partial B} = -\frac{2}{2\pi} \int_A^B \partial_B R(\alpha; A, B) \, d\alpha - \frac{2}{2\pi} R(B; A, B)$$

For the field, after using (8) and (11)

$$-4i \frac{\partial h}{\partial A} = -\frac{1}{2\pi} \int_A^B d\beta \, \partial_A R(\beta; A, B)[\Theta(A - \beta) + \Theta(B - \beta)]$$

$$+ R(A; A, B) \left[1 + \frac{1}{2\pi} \Theta(B - A) \right]$$

$$-4i \frac{\partial h}{\partial B} = -\frac{1}{2\pi} \int_A^B d\beta \, \partial_B R(\beta; A, B)[\Theta(A - \beta) + \Theta(B - \beta)]$$

$$+ R(B; A, B) \left[1 + \frac{1}{2\pi} \Theta(B - A) \right]$$

and finally

$$\frac{\partial F_R}{\partial A} = \frac{1}{2\pi} \int_A^B d\alpha \, \partial_A R(\alpha; A, B) \, f_R(\alpha; u) - \frac{1}{2\pi} R(A; A, B) \, f_R(A; u) + \frac{\partial h}{\partial A}$$

$$\frac{\partial F_R}{\partial B} = \frac{1}{2\pi} \int_A^B d\alpha \, \partial_B R(\alpha; A, B) \, f_R(\alpha; u) + \frac{1}{2\pi} R(B; A, B) \, f_R(B; u) + \frac{\partial h}{\partial B}$$

To evaluate the last two equations it is useful to know the branch cut structure of $f_R(\alpha; u)$. The cuts run from $i(\gamma - 2u)$ to $+i\infty$ and from $-i(\gamma + 2u)$ to $-i\infty$. The transition from the "A_R regime" to the "A_L regime" occurs when the integration path crosses the branch cut at $i(\gamma - 2u)$, since $f_L(\alpha; u)$ has a branch cut also starting from $i(\gamma - 2u)$ but running all the way down to $-i\infty$. Furthermore $\mathrm{Im}\, f_R(A_0; u) = \pi$ and $\mathrm{Im}\, f_R(B_0; u) = -\pi$.

It is now obvious how to go on by taking derivatives. The expansion has been carried out up to the third order. The variation of each quantity is a third order polynomial in δa, δb. It is convenient to introduce a more compact notation that brings out the geometrical meaning of the coefficients involved. Define

$$h_t(b) = \frac{d}{db} \bar{h}(b) = -\frac{1}{2} - \sum_{n=1}^{+\infty} (-)^n \frac{\cosh nb}{\cosh n\gamma} = -\frac{I(k)}{\pi} \mathrm{dn}\left(I + \frac{iIb}{\pi}; k\right)$$

where we have used (16) to express the series at hand as elliptic functions. For $\bar{v}(b)$ one has to distinguish between the two cases $b > \gamma - 2u$ or $b < \gamma - 2u$, but the elliptic function expression is the same for both cases

$$v_t(b) = \frac{d}{db} \bar{v}(b) = \frac{I(k)}{\pi} \mathrm{dn}\left(I + \frac{iI}{\pi}(2u + b); k\right)$$

We will also need

$$h_1(b) = \frac{dh_t}{db} = ik^2 \left(\frac{I(k)}{\pi}\right)^2 \mathrm{sn}\left(I + \frac{iIb}{\pi}; k\right) \mathrm{cn}\left(I + \frac{iIb}{\pi}; k\right)$$

$$v_1(b) = \frac{dv_t}{db} = -ik^2 \left(\frac{I(k)}{\pi}\right)^2 \mathrm{sn}\left(I + \frac{iI}{\pi}(b + 2u); k\right) \mathrm{cn}\left(I + \frac{iI}{\pi}(b + 2u); k\right)$$

h_t is negative in the interval $-\gamma < b < \gamma$, and vanishes when $b = \pm\gamma$. At these two points, the tangent to Γ is parallel to the v-axis. Instead, $v_t = 0$ when $b = \gamma - 2u$. At this point the tangent to Γ is parallel to the h-axis.

There is of course another point of this kind on the other half of Γ, obtained by the symmetry $(h, v) \rightarrow (-h, -v)$. Finally it is proven in Appendix A that the combination $v_t h_1 - v_1 h_t$, that will appear later, is definite negative. For polarization and horizontal field one has

$$\delta y = \frac{h_t}{\pi} \delta a - \frac{h_t x_0}{2\pi} \delta a^2 + \frac{h_1}{\pi} \delta a \, \delta b$$

$$+ \frac{1}{2\pi} \left(\frac{h_t x_0^2}{2} - \frac{x_3}{3} \right) \delta a^3 - \frac{h_1 x_0}{2\pi} \delta a^2 \, \delta b + \frac{x_3}{2\pi} \delta a \, \delta b^2 \qquad (24)$$

$$\delta h = h_t \, \delta b - \frac{h_1}{2} \delta a^2 + \frac{h_1}{2} \delta b^2 - \frac{h_t x_0}{2} \delta a \, \delta b$$

$$- \frac{h_1 x_0}{6} \delta a^3 - \frac{x_3}{2} \delta a^2 \, \delta b + \frac{x_3}{6} \delta b^3 \qquad (25)$$

whereas, if we set $Z_0 = Z(\gamma - |\gamma - 2u - b|)/2\pi$

$$\delta F = -2h_t Z_0 \, \delta a + h_t x_0 Z_0 \, \delta a^2 - \left(2h_1 Z_0 + \frac{h_t v_t}{\pi} \right) \delta a \, \delta b$$

$$+ \left[\frac{2h_1 v_t}{\pi} + \frac{h_t v_1}{\pi} + Z_0(-3h_t x_0^2 + 2x_3) \right] \frac{\delta a^3}{6}$$

$$+ \left(\frac{h_t v_t x_0}{2\pi} + h_1 x_0 Z_0 \right) \delta a^2 \, \delta b$$

$$- \left(\frac{h_1 v_t}{\pi} + \frac{h_t v_1}{2\pi} + Z_0 x_3 \right) \delta a \, \delta b^2 \qquad (26)$$

Here x_0 and x_3 are non-zero terms that play little role in what follows

$$x_0 = \frac{1}{\pi} \left(1 + 2 \sum_{n=1}^{+\infty} \frac{e^{-n\gamma}}{\cosh n\gamma} \right)$$

$$x_3 = - \sum_{n=1}^{+\infty} (-)^n n^2 \frac{\cosh nb}{\cosh n\gamma} = \left(\frac{I(k)}{\pi} \right) \frac{d^2}{d\alpha^2} \, \mathrm{dn} \left(\frac{I(k) \, \alpha}{\pi}; k \right) \Big|_{\alpha = \pm \pi + ib}$$

What actually has to be minimized though is $\mathscr{F} = -F - vy$. Using (21) and (26)

$$\delta\mathscr{F} = -\delta F - \bar{v}(b)\,\delta y - \delta v\,\delta y = -\delta v\,\delta y + \frac{h_t v_t}{\pi}\,\delta a\,\delta b$$

$$-\left(\frac{h_t v_1}{\pi} + \frac{2h_1 v_t}{\pi}\right)\frac{\delta a^3}{6} + \left(\frac{h_1 v_t}{\pi} + \frac{h_t v_1}{2\pi}\right)\delta a\,\delta b^2$$

$$+\frac{x_0 v_t h_t}{2\pi}\,\delta a^2\,\delta b \qquad (27)$$

These expansions reduce to those of ref. 8 when $b \to \pm\gamma$ (the limit should be taken in the elliptic functions because several series are not convergent when $|b| = \gamma$). No term δb^n appears in (24), and that had to be expected since the line $a = \pi$ (i.e. $\delta a = 0$), $-\gamma \leqslant b \leqslant \gamma$ corresponds to $y = 0$. Furthermore, while (8) and following equations make perfectly sense for any values of A and B, one might object that solutions of (6) can always be taken to have $-\pi \leqslant \mathrm{Re}\,\alpha \leqslant \pi$. Hence a should vary in $[0, \pi]$. The question at issue is what solutions (6) admit when $n > N/2$, knowing that, when $n = N/2$, they already fill a line stretching from $-\pi$ to π. Fortunately, the question can be bypassed. Only variations $\delta v > 0$ will be considered and it is physically clear that $\delta v > 0$ tends to align arrows "up," therefore brings $\delta y > 0$, that is $n < N/2$ and, from (24), $\delta a < 0$. This is sufficient because only the upper half of Γ, given by (17), (21) is being considered. The other half, where to drive the system into the incommensurate phase one needs a variation $\delta v < 0$, can, as usual, be recovered from $f(h, v) = f(-h, -v)$.

4. MINIMIZATION OF $\mathscr{F}$ AND FREE ENERGY SINGULARITY

The minimum of $\mathscr{F}$ should now be taken with respect to y, when y, u, h, v are kept fixed. Keeping δh fixed at a given value means that δa and δb are not independent. Two different ways will be followed to deal with (24), (25) and (27) and they give the same results.

Neglecting terms $\delta a^3, \delta b^3$ in (25) and solving for δb one finds

$$\delta b = \frac{\delta h}{h_t} - \frac{h_1}{2h_t}\,\delta a^2 - \frac{h_1}{2h_t^3}\,\delta h^2 + \frac{x_0}{2h_t}\,\delta a\,\delta h + O(\delta a^3, \delta a^2\,\delta h, \delta a\,\delta h^2, dh^3) \qquad (28)$$

when inserted into $\delta \mathscr{F}$, one gets

$$\delta \mathscr{F} = \delta a \left(-\frac{h_t}{\pi} \delta v - \frac{h_1}{h_t \pi} \delta v \, \delta h + \frac{v_t}{\pi} \delta h + \frac{v_1 h_t + h_1 v_t}{2\pi h_t^2} \delta h^2 + \cdots \right)$$
$$+ \delta a^2 \left(\frac{h_t x_0}{2\pi} \delta v + c_2 \delta h^2 + \cdots \right) + \frac{\delta a^3}{6\pi} \Delta + \cdots \tag{29}$$

$$\Delta = v_t h_1 - v_1 h_t \tag{30}$$

All terms neglected are higher order, i.e. δa^4, $\delta a^3 \delta h$, $\delta a^2 \delta v \, \delta h^2$, $\delta a \, \delta v \, \delta h^2$, etc. and it will soon become clear that dropping them is justified. The coefficient c_2 is b-dependent and to know its specific value will not be necessary in the following.

Let's consider the coefficient of δa in (29). It is easy to see, from (17) and (21) that it vanishes when the variation $(\delta h, \delta v)$ is taken along Γ. This had to be expected. The curve Γ is described by minima of $\mathscr{F}$ falling on the line $a = \pi$, $-\gamma \leqslant b \leqslant \gamma$ or, stated otherwise, with $\delta a = 0$. In fact, the vanishing of the first order term in (29) implies that $\delta \mathscr{F}$ has a stationary point at $\delta a = 0$. Suppose next that we approach Γ along any direction other than the tangential one, that is

$$\delta v = k \, \delta h \qquad k \neq \frac{v_t}{h_t} \tag{31}$$

To move into the incommensurate phase one has to take $\delta h > 0$ for $k > v_t/h_t$ and $\delta h < 0$ for $k < v_t/h_t$. Clearly the linear terms in the coefficient of δa in (29) do not cancel and therefore the terms $\delta v \, \delta h$, δh^2 (and higher) in the same coefficient can be dropped. Same thing can be said about the δa^2 term since, obviously, $\delta a^2 \ll \delta a$. The term δa^3 must be retained in all cases, because its coefficient is finite. Instead terms like $\delta a^3 \delta h$, δa^4 etc. are clearly negligible compared with the δa^3 term. It can be seen by inspection that the terms thrown away in solving (25) are also negligible. The whole procedure assumes though that a small variation $(\delta h, \delta v)$ brings about a small displacement $(\delta a, \delta b)$ in the minimum of $\mathscr{F}$. The upshot is that it is legitimate to keep

$$\delta \mathscr{F} = \frac{\delta a^3}{6\pi} \Delta + \delta a \left(-\frac{h_t}{\pi} \delta v + \frac{v_t}{\pi} \delta h \right) \tag{32}$$

Once (31) is taken into account, the solution of

$$\frac{\partial \delta \mathscr{F}}{\partial \delta a} = 0$$

occurs at

$$\delta a_0 = -\left[\frac{2(kh_t - v_t)\,\delta h}{\Delta}\right]^{1/2} \tag{33}$$

Notice that the previous limits on k guarantee that the solution is real. The sign has been chosen to make sure that $\delta a < 0$. An elementary check shows that $\partial^2(\delta\mathscr{F})/\partial(\delta a)^2|_{\delta a_0} > 0$ and it confirms that δa_0 is a minimum. When δa_0 is plugged into (29) one finds that, when $\delta v = k\,\delta h$, $k \neq v_t/h_t$

$$\delta f = f(\gamma, u, h + \delta h, v + \delta v) - f_0(\gamma, u) = \left(\frac{h_t}{\Delta}\right)^{1/2}\frac{h_t}{3\pi}\left[2\left(k - \frac{v_t}{h_t}\right)\delta h\right]^{3/2} \tag{34}$$

So the exponent is 3/2 for all these directions. We pass next to the case where the transition line is approached tangentially, i.e.

$$\delta v = \frac{v_t}{h_t}\,\delta h$$

We have then

$$\delta\mathscr{F} = \frac{\delta a^3}{6\pi}\Delta + \frac{v_t x_0}{2\pi}\,\delta h\,\delta a^2 - \delta a\,\delta h^2\frac{\Delta}{2\pi h_t^2} \tag{35}$$

The minimum lies at

$$\delta a_0 = -\left[v_t x_0\,\delta h + \frac{|\delta h|}{h_t}\sqrt{\Delta^2 + (v_t h_t x_0)^2}\right]\bigg/\Delta \tag{36}$$

Since $\partial^2(\delta\mathscr{F})/\partial(\delta a)^2|_{\delta a_0} > 0$, δa_0 is indeed a minimum. Inserting it into $\delta\mathscr{F}$ yields a jump in the third derivative of the free energy. Namely, at $h_t\,\delta v = v_t\,\delta h$

$$\delta f = f(\gamma, u, h + \delta h, v + \delta v) - f_0(\gamma, u) = \begin{cases} c_+\,\delta h^3 & \text{if}\quad \delta h > 0 \\ c_-\,\delta h^3 & \text{if}\quad \delta h < 0 \end{cases} \tag{37}$$

where

$$c_\pm = \frac{1}{6\pi h_t^3\,\Delta^2}(g \pm \sqrt{g^2 + \Delta^2})(g^2 + 2\,\Delta^2 \pm g\sqrt{g^2 + \Delta^2}) \qquad g = v_t x_t x_0 \tag{38}$$

When $2u + b = \gamma$, $v_t = 0$. Then (38) somewhat simplifies, since $g = 0$ and the variation tangential to Γ is just δh, so

$$\delta f = -\frac{|v_1|}{3\pi h_t^2} |\delta h|^3$$

An analogous result, with $\delta v \leftrightarrow \delta h$ was reached in ref. 8, but only for the two points $b = \pm\gamma$, where the tangent to Γ is parallel to the v-axis

A second method of calculation will now be presented. From (15), the equation determining the equilibrium value of y is

$$\frac{\partial F}{\partial y}\bigg|_h + v = 0 \tag{39}$$

Equation (20) is just a particular case of this condition. It identifies the value of v for which the minimum occurs at $y = 0$. If one thinks to invert (15), (24), F becomes a function of a, b, so[2]

$$-v = \frac{\partial F}{\partial a}\bigg|_b \frac{\partial a}{\partial y}\bigg|_h + \frac{\partial F}{\partial b}\bigg|_a \frac{\partial b}{\partial y}\bigg|_h = \frac{(\partial F/\partial b)(\partial h/\partial a) - (\partial F/\partial a)(\partial h/\partial b)}{(\partial h/\partial a)(\partial y/\partial b) - (\partial h/\partial b)(\partial y/\partial a)} \tag{40}$$

which makes sense if (24) and (25) are indeed invertible, that is if the denominator in the RHS does not vanish. It is immediate to see from (24), (25) that this is true for the points we are considering. Instead, the points $b = \pm\gamma(h_t = 0)$ are saddle points for $h(a, b)$.[8] Expanding the denominator in (40) and retaining terms up to the second order (to have the third order in (40) one should expand y, h and F to the fourth order)

$$-v = -2\pi Z_0 - v_t \,\delta b + \frac{v_1}{2} \,\delta a^2 - \frac{v_1}{2} \,\delta b^2 - \frac{x_0 v_t}{2} \,\delta a \,\delta b$$

Writing $v = \bar{v}(b) + \delta v$, owing to (21) one arrives at

$$\delta v = v_t \,\delta b - \frac{v_1}{2}(\delta a^2 - \delta b^2) + \frac{v_t x_0}{2} \,\delta a \,\delta b + \cdots \tag{41}$$

$$\delta h = h_t \,\delta b - \frac{h_1}{2}(\delta a^2 - \delta b^2) - \frac{h_t x_0}{2} \,\delta a \,\delta b + \cdots \tag{42}$$

whose solution yields $\delta a(\delta h, \delta v)$ and $\delta b(\delta h, \delta v)$. Their result has to be used in (29) to produce the leading singular part of δf. Again, two cases have to be distinguished.

If $\delta v = k\,\delta h$, $k \neq v_t/h_t$, consistency of (40), (41) requires that $\delta b \sim c\,\delta a^2 + o(\delta a^2)$, so at the leading order

$$\delta v = \left(cv_t - \frac{v_1}{2} \right) \delta a^2$$

$$\delta h = \left(ch_t - \frac{h_1}{2} \right) \delta a^2$$

Hence

$$c = \frac{1}{2} \frac{v_1 - kh_1}{v_t - kh_t} \qquad \delta a = -\left[\frac{2(kh_t - v_t)\,\delta h}{\Delta} \right]^{1/2}$$

which coincides with (33). $\delta\mathscr{F}$ is obviously the same previously used, so the free energy coincides with (34). Suppose instead $\delta v = k\,\delta h$ but $k = v_t/h_t$. Clearly (41), (42) give $\delta b = \delta h/h_t$ at the leading order and

$$\Delta\delta a^2 + 2v_t x_0\,\delta a\,\delta h - \Delta\,\frac{\delta h^2}{h_t^2} = 0$$

whose solution is, again (36). Yet, replacing $\delta b = \delta h/h_t$ and (36) into (27) is not correct. The reason is that a term $\delta a\,\delta b$ appears in (27) that would require solving (41) and (42) for δb up to the next order in δh. The problem can be bypassed by replacing e.g. (42) into the term $\delta a\,\delta b$ of (27). So one gets

$$\delta\mathscr{F} = \frac{\delta a^3}{6\pi}\,\Delta + \frac{x_0 v_t}{2\pi}\,\delta h\,\delta a^2 - \frac{v_t h_1}{\pi h_t}\,\delta h\,\delta a\,\delta b + \frac{\delta a\,\delta b^2}{2\pi}\,(h_1 v_t + h_t v_1)$$

and after setting $\delta b = \delta h/h_t$ one is back to (35) and, because of (36), to the δf of (37).

APPENDIX

One has to prove that $\Delta < 0$ for all b in $(-\gamma, \gamma)$. Setting

$$x = I + \frac{iIb}{\pi} \qquad y = I + \frac{iI}{\pi}(b + 2u)$$

from (30)

$$\Delta = \left(\frac{I}{\pi} \right)^3 ik^2\,\mathrm{dn}(x; k)\,\mathrm{dn}(y; k) \left[\frac{\mathrm{sn}(x; k)\,\mathrm{cn}(x; k)}{\mathrm{dn}(x; k)} - \frac{\mathrm{sn}(y; k)\,\mathrm{cn}(y; k)}{\mathrm{dn}(y; k)} \right]$$

Perform Landen's transform[14]

$$k \to k_1 = \frac{1-k'}{1+k'} \qquad u \to u_1 = (1+k')u$$

$$\mathrm{sn}(u_1; k_1) = \frac{k}{k_1^{1/2}} \frac{\mathrm{sn}(u; k)\,\mathrm{cn}(u; k)}{\mathrm{dn}(u; k)}$$

The new half-periods are

$$I_1 = I(k_1) = \frac{1+k'}{2} I(k) \qquad I_1' = I'(k_1) = (1+k')\,I'(k)$$

and so

$$\varDelta = k_1^{1/2} ik \left(\frac{I}{\pi}\right)^3 \mathrm{dn}(x; k)\,\mathrm{dn}(y; k)\left[\mathrm{sn}\left(\frac{iI_1'}{\gamma}(b+2u); k_1\right) - \mathrm{sn}\left(\frac{iI_1'b}{\gamma}; k_1\right)\right]$$

A table of signs of dn, cn and sn is given in ref. 14. By inspecting the possible cases one sees that $\varDelta < 0$ always. A possible exception comes from $\mathrm{dn}(y; k) = 0$ that is when $b + 2u = \gamma$. In this case $v_t = 0$ and

$$\varDelta = -v_1 h_t(b = \gamma - 2u) = h_t k' \left(\frac{I}{\pi}\right)^2 < 0$$

There might be a simpler proof.

ACKNOWLEDGMENTS

REFERENCES

1. C. P. Yang, *Phys. Rev. Lett.* **19**:586 (1967); B. Sutherland, C. N. Yang and C. P. Yang, *Phys. Rev. Lett.* **19**:588 (1967).
2. I. M. Nolden, *J. Stat. Phys.* **67**:155 (1992) and Ph.D. dissertation.
3. M. Gaudin, in *La fonction d'onde de Bethe* (Masson, Paris, 1983).
4. E. H. Lieb and F. Y. Wu, in *Phase Transitions and Critical Phenomena*, ed. C. Domb and M. S. Green, vol. 1 (Academic Press, London, 1972).
5. J. D. Noh and D. Kim, *Phys. Rev. E* **53**:3225 (1996).

6. D. Kim, *J. Phys.* **A30**:3817 (1997).
7. G. Albertini, S. Dahmen, and B. Wehefritz, *J. Phys. A* **29**:L369 (1996).
8. G. Albertini, S. Dahmen, and B. Wehefritz, *Nucl. Phys. B* **493** [FS]:541 (1997).
9. V. L. Pokrovski and A. L. Talapov, *Sov. Phys. JETP* **51**:134 (1980).
10. M. den Nijs, in *Phase Transitions and Critical Phenomena*, ed. C. Domb and J. Lebowitz, vol. 12 (Academic Press, London, 1988).
11. N. M. Bogoliubov, A. G. Izergin, and V. E. Korepin, *Nucl. Phys. B* **275** [FS]:687 (1986).
12. R. J. Baxter, *Exactly Solvable Models in Statistical Mechanics*, (Academic Press, London, 1982).
13. F. R. Gantmacher, in *Matrix Theory* (Chelsea, New York, 1959)
14. A. Erdélyi *et al.* ed., *Higher Trascendental Functions* vol. 2 (McGraw-Hill, New York, 1953).
15. H. van Beijeren, *Phys. Rev. Lett.* **38**:993 (1977).
16. C. Jayaprakash, W. F. Saam, and S. Teitel, *Phys. Rev. Lett.* **50**:2017 (1983); C. Jayaprakash and W. F. Saam, *Phys. Rev. B* **30**:3916 (1984).