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EXACT SOLUTION OF A MODEL OF TWO-DIMENSIONAL FERROELECTRICS IN AN ARBITRARY EXTERNAL ELECTRIC FIELD

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This paper summarizes the main features of the exact solution of the model discussed by Yang,[1] which is the last of a series of generalizations[2,3] of Lieb's solution[4] of the ice problem.

Integral equation.—We can choose

$$\delta > 0, \tag{1}$$

i.e., $\eta \geqslant 1$ without loss of generality.

To find the partition function, one first considers (Y7). The solution of this equation is such that as $N \to \infty$, the points $z_j = H \exp(ip_j) = \exp(ip_j^0)$ $(j = 1, 2, \cdots, m)$ arrange themselves along a smooth curve C in the complex z plane. The curve C is symmetrical with respect to the transformation $z \leftrightarrow z^*$. Denote the two ends of the curve C by Z and Z^* with Z in the upper-half complex plane. The number of z_j's in any interval dz along C is $N\rho(p^0)dp^0$. Let f be such that along C,

$$df/dp^0 = \rho(p^0) \tag{2}$$

with $f = 0$ at the midpoint of C. Then

$$p^0 = (-i \ln H + 2\pi f) - \int_C \Theta(p^0, q^0)\, \rho(q^0) dq^0, \tag{3}$$

where Θ is a function defined by Yang and Yang.[5] Notice that (3) reduces to (II 3) of Ref. 5 when $H = 1$.

Equation (3) defines f as a function of p^0 when z is continued analytically away from C. Differentiation with respect to p^0 gives

$$2\pi\rho = 1 + \int_C (\partial\Theta/\partial_p{}^0)(p^0, q^0)\rho(q^0)dq^0, \tag{4}$$

which is identical in form with the integral equation (II 6a), except for the difference of the path of integration.

For given end points Z and Z^*, (4) in general has a unique solution. Substitution of the solution into (3) yields the function g, where

$$2\pi g = 2\pi f - i \ln H. \tag{5}$$

The value of g at the end point Z is known since that of f is known at that point. We have, in fact,

$$2\pi g(Z) = \tfrac{1}{2}\pi(1-y) - i \ln H, \tag{6}$$

which is the generalization of (II 6b).

The Curve C is defined by those points z at which

$$-\mathrm{Im}\, 2\pi g = \ln H \tag{7}$$

between the end points Z and Z^*.

The integral equation (4) and the relation (6) are best studied after a transformation $p_0 \to \alpha$ which was explicitly given in (I21) for the cases $\Delta < -1$ (λ region), $\Delta = -1$, and $-1 < \Delta < 1$ (μ region). [One writes p_0 for all p in (I21).] For the present problem, we need similar transformations in the additional cases of $\Delta = +1$ and $1 < \Delta$. For

$$\Delta = +1, \quad \exp(ip^0) = \frac{1 + 2i\alpha}{-1 + 2i\alpha}; \tag{8a}$$

$$1 < \Delta, \quad \exp(ip^0) = \frac{e^{\nu} - e^{-i\alpha}}{-e^{\nu - i\alpha} + 1}, \quad \Delta = \cosh\nu, \quad \nu > 0. \tag{8b}$$

The end points Z and Z^* are mapped in the complex α plane into $(b + i\Phi)$ and $(-b + i\Phi)$. For given b and Φ, the integral equation (4) then becomes a nonsingular Fredholm equation. Evaluation of ρ, and then g from (3), yield through (6) the values of y and H. Thus y and H are real functions of the real variables b and Φ.

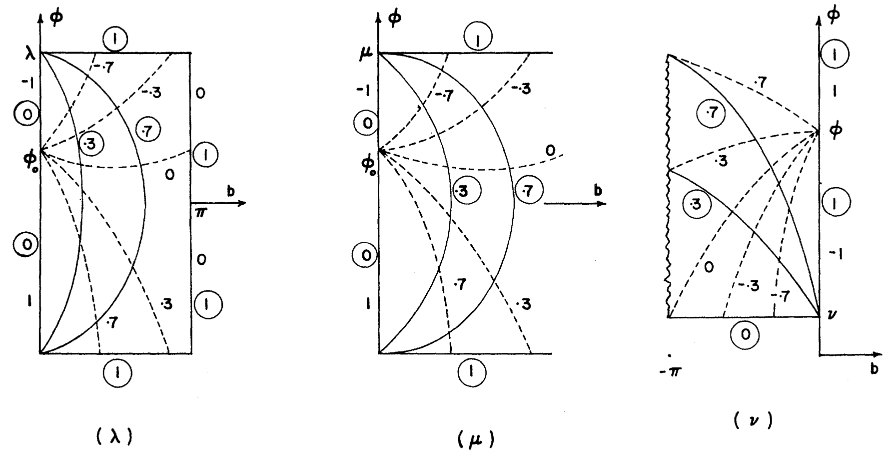

FIG. 1. Schematic diagram of constant-x and -y contours in b-Φ plane. Dotted lines are constant-x contours with x values given. Solid lines are constant-y contours with y values given in circles. In the λ and μ regions all values of x,y satisfying $-1\leq x\leq 1, 0\leq y\leq 1$ are attained in the b-Φ diagram shown. In the ν region, only those values of x and y satisfying the further condition $y\geq x$ are attained in the b-Φ diagram shown. The diagram for $\Delta=-1$ is similar to that of the μ region, except that the label μ at the corner should be changed to read $\Phi=\frac{1}{2}$. The diagram for $\Delta=+1$ is similar to that of the ν region, except that the label ν at the corner should be changed to read $\Phi=\frac{1}{2}$ and the wavy left-side boundary should be pushed to $b=-\infty$.

The region of b and Φ of interest is shown in Fig. 1 with some important special points located.

Evaluation of the thermodynamic function.— The two terms of (Y6) can be separately evaluated. It can be proved that the bigger of the two is given by an integration along a path D which is not necessarily C, giving

$$-F_{hy}/N^2kT=\tfrac{1}{2}\ln\eta+\tfrac{1}{2}\ln H+\int_D \ln\left[\eta^{-1}-\frac{\xi}{1-\eta\exp(ip^0)}\right]\rho(p^0)dp^0, \tag{9}$$

where D starts from Z^*, ends at Z, and passes the real axis in the z plane at a point $z=z_1>\eta^{-1}$.

Results.— Detailed investigation of (4), (3), (6), and (9) leads to the complete thermodynamical properties of the model. We summarize the most important features below:

(A) The thermodynamic function $F_{xy}(T,x,y)$ is defined for all T on the square $-1\leq x\leq 1$, $-1\leq y\leq 1$. It satisfies the symmetry conditions (Y18). It is a continuous function of T, x, and y and concaves upwards in the double variables x and y. The horizontal and vertical fields h and v are the derivatives of F_{xy}: $N^{-2}dF_{xy}=-sdT+hdx+vdy$ (Y15).

(B) Near $y=1$, $x\neq\pm1$, F_{xy} can be expanded and the first two terms are as exhibited in the following equation:

$$N^{-2}F_{xy}=-\tfrac{1}{2}x\delta+kT(1-y)\{-\tfrac{1}{2}-\tfrac{1}{2}\ln\xi+\tfrac{1}{2}\ln[\tfrac{1}{2}\pi(1-y)]-\tfrac{1}{2}\ln\cos\tfrac{1}{2}\pi x\}+\cdots. \tag{10}$$

Thus as $y\to 1$, $x=\text{fixed}\neq\pm1$, $v\to+\infty$ logarithmically.

(C) F_{xy} is analytic in T, x, and y everywhere in the open square $0<T<\infty$, $-1<x<1$, $-1<y<1$, except for (i) the points

$$x=y,\quad \Delta\geq 1; \tag{11}$$

(ii) the points

$$x=y=0,\quad -1\leq\Delta\leq 1; \tag{12}$$

and (iii) the points

$$x=y=0,\quad \Delta<-1. \tag{13}$$

(D) The value of $N^{-2}F_{xy}$ at the singular points (11)-(13) is

$$N^{-2}F_{xy}(x,x) = -\tfrac{1}{2}\delta, \quad 1 \leq \Delta; \tag{14}$$

$$N^{-2}F_{xy}(0,0) = -\frac{1}{2}\delta - \frac{kT}{8\mu}\int_{-\infty}^{\infty}\frac{d\alpha}{\cosh(\pi\alpha/2\mu)}\ln\left[\frac{\cosh\alpha-\cos(2\mu-\Phi_0)}{\cosh\alpha-\cos\Phi_0}\right], \quad -1<\Delta<1; \tag{15}$$

$$N^{-2}F_{xy}(0,0) = -\tfrac{1}{2}\delta - kT\sum_1^{\infty}(-1)^n \ln[(n\eta+n-1)(n\eta+n+1)^{-1}], \quad \Delta = -1; \tag{16}$$

$$N^{-2}F_{xy}(0,0) = -\frac{1}{2}\delta - kT\left\{\frac{1}{2}\lambda - \frac{1}{2}\Phi_0 + \sum_1^{\infty}\frac{e^{-\lambda n}\sinh[n(\lambda-\Phi_0)]}{n\cosh n\lambda}\right\}, \quad \Delta < -1. \tag{17}$$

In these formulas λ and μ are defined as in I, and Φ_0 is defined so that $\alpha = i\Phi_0$ corresponds to $\exp(ip^0) = \eta^{-1}$:

$$e^{\Phi_0} = \frac{1+e^{\lambda}\eta}{e^{\lambda}+\eta}, \quad 0 \leq \Phi_0 \leq \lambda; \tag{18a}$$

$$e^{i\Phi_0} = \frac{1+\eta e^{i\mu}}{e^{i\mu}+\eta}, \quad 0 \leq \Phi_0 \leq \mu; \tag{18b}$$

$$e^{\Phi_0} = \frac{\eta e^{\nu}-1}{\eta - e^{\nu}}, \quad \nu \leq \Phi_0; \tag{18c}$$

$$\Phi_0 = \frac{1}{2}\frac{\eta-1}{\eta+1}, \text{ for } \Delta=-1, \quad 0 \leq \Phi_0 \leq \tfrac{1}{2}; \tag{18d}$$

$$\Phi_0 = \frac{1}{2}\frac{\eta+1}{\eta-1}, \text{ for } \Delta=+1, \quad \tfrac{1}{2} \leq \Phi_0. \tag{18e}$$

Notice that in (18c), it follows from $2\cosh\nu = \eta + 1/\eta - \xi$ that $\eta > e^{\nu}$.

(E) For $1 \leq \Delta$, along the line $x=y$, the function $N^{-2}F_{xy}$ has the constant value $-\frac{1}{2}\delta$. In the neighborhood of this line F_{xy} has one tangent plane for $x=y+0$ and a different one for $x=y-0$, so that

$$h = -v = \pm\tfrac{1}{2}kT\nu \tag{19}$$

at $x=y\pm0$. The line $x=y$ is thus a groove for the function F_{xy}.

(F) For $-1 \leq \Delta < 1$, the function $N^{-2}F_{xy}(x,y)$ has a singularity only at $x=y=0$, if at all. In the neighborhood of this point,

$$N^{-2}F_{xy}(x,y) = N^{-2}F_{xy}(0,0) + \frac{\pi-\mu}{4\cos(\Phi_0\pi/2\mu)}[x^2+y^2-2xy\sin(\Phi_0\pi/2\mu)] + \text{higher order terms.} \tag{20}$$

Higher derivatives than the second with respect to x and y sometimes become $\pm\infty$ as x and $y \to 0$.

(G) For $\Delta < -1$, the function $N^{-2}F_{xy}(x,y)$ has a conical singularity at $x=y=0$, at which F_{xy} does not have a unique tangent plane. In fact the single point $x=y=0$ corresponds to a region in the h-v plane. The region is bounded by the closed curve $(-2\lambda \leq \Phi \leq 2\lambda)$:

$$h = -kTZ(\Phi), \tag{21}$$

$$v = kTZ(\lambda - \Phi_0 + \Phi), \tag{22}$$

where $Z(\Phi)$ is an odd function of Φ, analytic for all real Φ, and

$$Z(\Phi) = \frac{1}{2}\Phi + \sum_1^{\infty}\frac{(-1)^n\sinh n\Phi}{n\cosh n\lambda}, \quad -\lambda < \Phi < \lambda. \tag{23}$$

It is easy to prove that

$$Z(\lambda-\Phi)=Z(\lambda+\Phi), \tag{24}$$

$$Z(\Phi+4\lambda)=Z(\Phi), \tag{25}$$

and

$$dZ/d\Phi=\text{const}\times\text{the elliptic function nd}(\text{const}\times\Phi). \tag{26}$$

(H) The singularity discussed in (E) appears in $N^{-2}F_{hv}(h,v)$ as two plane segments: (i) For $h+v\geq 0$,

$$[-1+\eta\exp(2h/kT)][-1+\eta\exp(2v/kT)]\geq\eta\xi,\quad N^{-2}F_{hv}=-2^{-1}\delta-h-v.$$

(ii) For $h+v\leq 0$,

$$[-1+\eta\exp(-2h/kT)][-1+\eta\exp(-2v/kT)]\geq\eta\xi,\quad N^{-2}F_{hv}=-2^{-1}\delta+h+v.$$

The remaining two parts of the h-v plane have a functional value for $N^{-2}F_{hv}$ forming curved F-h-v surfaces. The complete F_{hv} vs h-v surface is thus like a roof with two plane parts joined by two curved ends.

(I) The singularity discussed in (G) appears in the $N^{-2}F_{hv}$ vs h-v surface as a flat bottom bounded by the curve (21)-(22). The whole surface is in the shape of an infinite bowl with a flat bottom.

(J) The special case $\Delta=0$ (i.e., $\mu=\frac{1}{2}\pi$) is simply solvable since the function Θ is zero. The result gives

$$2\sinh\frac{2h}{kT}=-\left(\eta-\frac{1}{\eta}\right)\sin\frac{1}{2}\pi y+\left(\eta+\frac{1}{\eta}\right)\cos\frac{1}{2}\pi y\tan\frac{1}{2}\pi x,\quad 2\sinh\frac{2v}{kT}=\text{same with } x\leftrightarrow y. \tag{27}$$

Previous models.—The F model and the KDP model solved[2,3] by Lieb and Sutherland correspond to the cases $\eta=1$ and $\eta=\xi^{-1}$, respectively. Wu's model[6] corresponds to taking the following limit in our considerations:

$$\Delta=0,\quad \eta\to\infty,\quad h+v=0,\quad h+\epsilon=\text{negative constant}.$$

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[1]C. P. Yang, preceding Letter [Phys. Rev. Letters 19, 000 (1967)]. Our notation follows that of this paper which will be referred to as Y. (Y7) means (7) of Y.

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[5]C. N. Yang and C. P. Yang, Phys. Rev. 150, 321, 327 (1966). These papers are referred to as I and II.

[6]F. Y. Wu, Phys. Rev. Letters 18, 605 (1967).