

can proceed to discuss the spectrum of  $H^-$  in this representation, but one is misled by so doing. The misconceptions that arise are caused by one's desire to label states  $\eta_{\phi^-}^{(-)\dagger}|0_-\rangle$ ,  $\phi^- \neq 0$ , as single-particle states and, correspondingly, single spin-wave states. However, they are not such states because  $\Lambda(0) < 0$ . It is better to transform  $\xi_{\phi^-} = \eta_{\phi^-}^{(-)}$  for  $\phi^- \neq 0$  and  $\xi_0^- = \eta_0^{(-)}$ . Then for  $h < 1$

$$H^- = |\Lambda(0)| \xi_0^{\dagger} \xi_0 + \sum_{\phi^- \neq 0} \Lambda(\phi^-) \xi_{\phi^-}^{\dagger} \xi_{\phi^-} . \quad (5.7)$$

Because of the change of basis, the even  $\xi$  excitations of  $H^-$  above the new vacuum  $|0'_-\rangle$  are eigenstates of  $H^-$ ; i.e., because

$$\exp\left(i\pi \sum_{\phi^-} \eta_{\phi^-}^{(-)\dagger} \eta_{\phi^-}^{(-)}\right) = -\exp\left(i\pi \sum_{\phi^-} \xi_{\phi^-}^{\dagger} \xi_{\phi^-}\right) , \quad (5.8)$$

evenness and oddness have switched.  $|0'_-\rangle$  is de-

finied by  $\xi_{\phi^-}|0'_-\rangle = 0$ , all  $\phi^-$ . It is now easily seen that the ground state of  $H$  is doubly degenerate with eigenstates  $|0_+\rangle$  and  $|0'_-\rangle$ . The first excited states of  $H$  consist of the two particle  $\eta^{(+)}$  excitations of  $H^+$  and the two-particle  $\xi$  excitations of  $H^-$ . These can be interpreted as two spin-wave states.

Therefore, for  $h > 1$  the ground state of  $H$  is non-degenerate with energy zero and is the ground state  $|0_+\rangle$  of  $H^+$ . The first excited states  $\eta_{\phi_+}^{(+)\dagger}|0_+\rangle$  ( $N$  single-particle states) come from  $H^+$  as given by (5.4) and are single spin-wave states with energy equal to  $\Lambda(\phi^+)$ .

For  $h < 1$  the ground state of  $H$  is doubly degenerate and consists of the ground states,  $|0_+\rangle$  and  $|0'_-\rangle$ , of  $H^+$  and  $H^-$ , respectively. The first excited states are the two-particle states,  $\eta_{\phi_+}^{(+)\dagger} \eta_{\phi_+}^{(+)\dagger}|0_+\rangle$  and  $\xi_{\phi_+}^{\dagger} \xi_{\phi_+}^{\dagger}|0'_-\rangle$ , of  $H^+$  and  $H^-$  as given by (5.3) and (5.7), respectively. There are  $N^2 - N$  such states, and they correspond to two spin-wave states.

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## Circle Theorem for the Ice-Rule Ferroelectric Models\*

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We show that the circle theorem on the distribution of zeros of the partition function breaks down for the ferroelectric potassium dihydrogen phosphate (KDP) model if the field lies outside the first quadrant. We also use a recent result by Suzuki and Fisher to establish the circle theorem for the antiferroelectric  $F$  model with a staggered electric field. Numerical results on the distribution of zeros for a  $4 \times 4$  lattice are given.

### INTRODUCTION

A central problem in the theory of phase transitions has been the investigation of the distribution of zeros of the partition function.<sup>1</sup> For the Ising ferromagnet in a magnetic field, Lee and Yang<sup>1</sup> showed that all zeros of the partition function lie on the unit circle, a result known as the "circle theo-

rem." This circle theorem has recently been extended to a number of other models.<sup>2</sup> One particular model which has been discussed is the ice-rule ferroelectric model of hydrogen-bonded crystals.<sup>3</sup> For the ferroelectric potassium dihydrogen phosphate (KDP) model Suzuki and Fisher<sup>2</sup> (SF) showed that all zeroes of the partition function with an electric field in the *first quadrant* lie on the unit circle

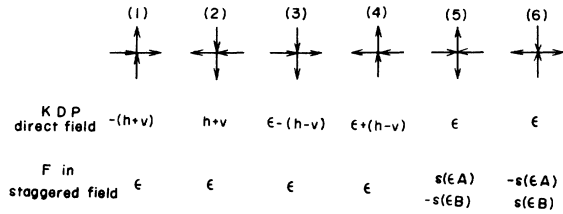


FIG. 1. Vertex configurations and energies of the KDP model in a direct electric field  $(h, v)$  and the  $F$  model in a staggered field. The staggered field varies sign from site to site (see text).

at temperatures below the transition temperature  $T_0$ . This result has been confirmed by numerical calculations carried out by Katsura, Abe, and Ohkouchi<sup>4</sup> (KAO) for finite lattices. KAO have also computed the zeros of the antiferroelectric  $F$  model in a direct field, and found that, in general, they do not lie on the unit circle. Two questions now arise: (i) Does the circle theorem hold for the ferroelectric KDP model with field outside the first quadrant? (ii) Is there a circle theorem for the  $F$  model in a staggered field? The second question is of importance because in an antiferroelectric model it is the staggered field which plays the role of a direct field in a ferroelectric model. We address ourselves to these two questions in the present paper.

CIRCLE THEOREM

To answer the first question we have carried out numerical studies on the partition function of a  $4 \times 4$  KDP lattice with an electric field in the *second quadrant*. Our result shows that the circle theorem does not hold in this case. In fact, it is easy to see the breakdown of the circle theorem by considering just a  $1 \times 1$  lattice. We remind the readers of the definition of the model as that given in Fig. 1.<sup>3</sup> Let us consider an electric field  $(h, v)$  in the second quadrant with  $h = -v$ . For a periodic  $1 \times 1$  lattice only the four vertices (1)–(4) are allowed, the par-

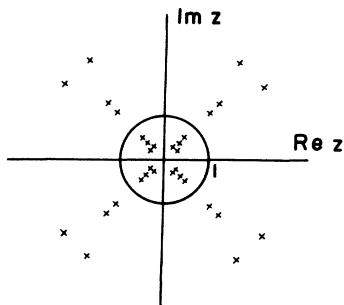


FIG. 2. Distribution of zeros for the  $4 \times 4$  KDP lattice with  $h = -v$  at  $\epsilon/kT = 0.7$  ( $T < T_0$ ).

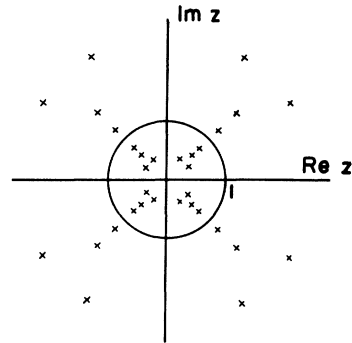


FIG. 3. Distribution of zeros for the  $4 \times 4$  KDP lattice with  $h = -v$  at  $\epsilon/kT = 0.5$  ( $T > T_0$ ).

tion function then takes the form

$$Z = 2 + \gamma(z + z^{-1}), \tag{1}$$

where  $\gamma = e^{-\beta\epsilon}$ ,  $z = e^{-2\beta v}$ . It is now easy to see that the zeros of  $Z$ ,  $z = -\gamma^{-1} \pm (\gamma^{-2} - 1)^{1/2}$ , do not lie on the unit circle. Thus we conclude by this counter example that in general the circle theorem does not hold for the KDP model if the field lies outside the first quadrant. Numerical results which confirm this conclusion for a  $4 \times 4$  KDP lattice will be given presently.

The second question can be answered affirmatively as follows. The  $F$  model with a staggered field is defined with the energy parameters as shown in Fig. 1. Notice that the vertices (5)–(6) have energies  $+s$  or  $-s$  depending on which sublattice,  $A$  or  $B$ , the vertex belongs. However, this model with position-dependent energies can be transformed into one with uniform energies. The trick is to reverse, in the enumeration of states, the arrow directions along every other zigzag path in the

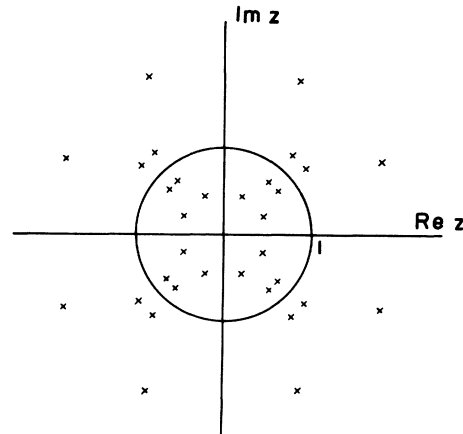


FIG. 4. Distribution of zeros for the  $4 \times 4$  KDP lattice with  $h = -v$  at  $\epsilon/kT = 0.1$  ( $T > T_0$ ).

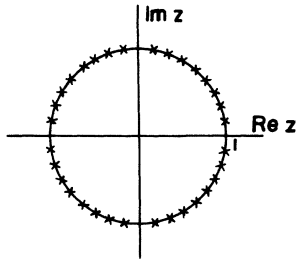


FIG. 5. Distribution of zeros for the  $4 \times 4$   $F$  lattice with a staggered field at  $\epsilon/kT = 0.7$  ( $T < T_0$ ).

northeast-southwest direction.<sup>5</sup> One then has an equivalent model with the following energy assignments:

$$\begin{aligned} e_1 = s, \quad e_2 = -s, \quad e_3 = e_4 = \infty, \\ e_5 = e_6 = e_7 = e_8 = \epsilon, \end{aligned} \quad (2)$$

where  $e_i$  is the energy of the  $i$ th vertex, and, in

$$\begin{aligned} Z_{\text{KDP}} = y^{16} (z^{16} + z^{-16}) + 8y^{12} (z^{12} + z^{-12}) + (4y^{16} + 48y^{14} + 124y^{12} + 16y^{10} + 12y^8) (z^8 + z^{-8}) \\ + (248y^{12} + 496y^{10} + 48y^8 + 8y^4) (z^4 + z^{-4}) + (6y^{16} + 96y^{14} + 432y^{12} + 496y^{10} + 288y^8 + 32y^6 + 2); \end{aligned} \quad (3)$$

$F$  with a staggered field,

$$\begin{aligned} Z_F = (z^{16} + z^{-16}) + 16y^4 (z^{12} + z^{-12}) + (140y^8 + 32y^6) (z^8 + z^{-8}) \\ + (256y^{12} + 384y^{10} + 144y^8) (z^4 + z^{-4}) + (256y^{16} + 640y^{12} + 384y^{10} + 152y^8). \end{aligned} \quad (4)$$

Introducing the variable

$$u = z^4 + z^{-4}, \quad (5)$$

we find

$$\begin{aligned} Z_{\text{KDP}} = y^{16} u^4 + 8y^{12} u^3 + (48y^{14} + 124y^{12} + 16y^{10} + 12y^8) u^2 \\ + (224y^{12} + 496y^{10} + 48y^8 + 8y^4) u + (184y^{12} + 496y^{10} + 288y^8 + 32y^6 + 2), \end{aligned} \quad (6)$$

$$\begin{aligned} Z_F = u^4 + 16y^4 u^3 + (140y^8 + 32y^6 - 4) u^2 + (256y^{12} + 384y^{10} + 144y^8 - 48y^4) u \\ + (256y^{16} + 640y^{12} + 384y^{10} - 128y^8 - 64y^6 + 2). \end{aligned} \quad (7)$$

These are quartic polynomials in  $u$ , and the zeros of  $Z$  can now be found by the solution of a quartic equation. The corresponding values of  $z$  can then be obtained by solving (5). Notice that since (5) involves only  $z^4$ , we have always at least four  $z$ 's locating on a circle. This is due to the periodic boundary condition imposed on the model which has

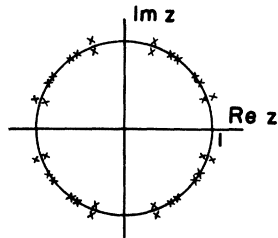


FIG. 6. Distribution of zeros for the  $4 \times 4$   $F$  lattice with a staggered field at  $\epsilon/kT = 0.5$  ( $T > T_0$ ).

addition to the vertex configurations (1)–(6) of Fig. 1, two new vertices [numbered (7) and (8)] with four arrows in or out are included. This model is however precisely a special case of the situation considered by SF with a direct field  $h = v = \frac{1}{2}s$  in the first quadrant.<sup>6</sup> The result of SF now establishes the following *circle theorem for the  $F$  model*.

The zeros of the  $F$  model in a staggered field lie on the unit circle for  $T < T_0$ , where  $T_0 = \epsilon/(k \ln 2)$  is the transition temperature.

#### NUMERICAL RESULTS

For a  $4 \times 4$  lattice, the zeros of the partition function in an external direct or staggered field can be obtained by the solution of a quartic equation. With  $y = e^{-\beta\epsilon}$ ,  $z = e^{-2\beta v}$ , or  $z = e^{-\beta s}$ , we find by explicit enumerations the following expressions for the partition function: for KDP with  $h = -v$ ,

the consequence of conserving the number of down arrows from row to row.<sup>3</sup> In Figs. 2–7 we present results on numerical calculations of the zeros of

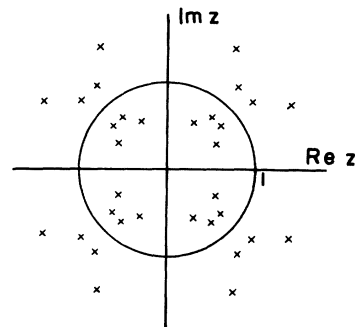


FIG. 7. Distribution of zeros for the  $4 \times 4$   $F$  lattice with a staggered field at  $\epsilon/kT = 0.1$  ( $T > T_0$ ).

$Z_{\text{KDP}}$  and  $Z_F$  for a  $4 \times 4$  lattice at three different temperatures,  $\epsilon/kT = 0.7, 0.5,$  and  $0.1$ . The transition temperature is located at  $\epsilon/kT_0 = \ln 2 = 0.693$ . Figure 6 confirms that the zeros of the  $F$  model in a staggered field lie on the unit circle for  $T < T_0$ . It is also to be noted that our variable  $z$  is related to the conventional fugacity variable  $\bar{z} = e^{-\beta v}$ , where  $\bar{v} = \sqrt{2}v$  is the magnitude of the applied field,

by the relation  $z = \bar{z}^{-\sqrt{2}}$ . Evidently  $|z| = 1$  implies  $|\bar{z}| = 1$ .

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<sup>6</sup>See Eq. (2.54) of Ref. 2.

## Integrodifferential Equation for Response Theory

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The problem of response theory in statistical mechanics involves the determination of the density matrix  $\rho$  from the Liouville equation and the subsequent computation of the response  $r$  from this  $\rho$ . Projection techniques are applied to avoid the entire complicated problem of the full dynamics of  $\rho$  and to select only that part of  $\rho$  which is relevant to the response  $r$ . The procedure replaces an inhomogeneous equation by a linear homogeneous integrodifferential equation for response theory. This is a very general equation which can be analyzed in different ways to yield a variety of results. It is shown that the Kubo theory of linear response emerges as the lowest-order approximation. The general equation is solved without approximations for a step-function stimulus, and it is discussed in the context of the steady state.

### I. INTRODUCTION

Response theory in physics has a very broad scope, and there is very little in physics that cannot be reformulated in its terms. Its concepts, however, are particularly useful in the treatment of problems of the nature of transport analysis. For this, one uses statistical mechanics, and a response theory essentially proceeds in the following three steps: (i) the determination of the density matrix  $\rho$  corresponding to the system in question, (ii) the incorporation of the stimulus  $s$  applied to the system in this determination, and (iii) the extraction of the required response  $r$  from the  $\rho$  thus determined.

The determination of  $\rho$  involves its time evolution, which is governed by

$$i \frac{\partial \rho(t)}{\partial t} = L(t)\rho(t), \quad (1)$$

where we write  $\hbar = 1$ , and  $L$  is the Liouville operator defined by

$$LO = [H_T, O] \quad (\text{for any operator } O), \quad (2)$$

with  $H_T$  as the Hamiltonian of the system with the stimulus applied to it. The stimulus thus appears through  $H_T$ .

The extraction of the response is easily accomplished through

$$r(t) = \text{Tr} R \rho(t), \quad (3)$$

where  $R$  is the operator (assumed for convenience to be time independent) corresponding to the response  $r$ . In Eq. (3) and from here on we do not display the factor  $(\text{Tr} \rho)^{-1}$  multiplying expressions like the right-hand side of Eq. (3).

The usual straightforward analysis therefore involves the complicated solution of the full dynamical problem presented by Eq. (1), followed by the