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# Two-dimensional frustrated Ising network as an eigenvalue problem

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The Pfaffian method is used to study the square frustrated Ising network. The formalism is adapted in order to develop a relation with the problem of excitations in random alloys. It is shown that the counterpart of frustrated plaquettes are local modes within a band gap. Properties of the local modes are examined, including questions of gauge invariance and duality. Numerical calculations are done to investigate the way in which the local modes broaden into an impurity band.

## I. INTRODUCTION

There has been considerable recent interest in the square ferromagnetic Ising network in which a fraction $p$ of the bonds are replaced by antiferromagnetic ones. The model represents the simplest frustrated system and it is thus supposed to be relevant to the spin-glass problem. It appears increasingly evident however, that no spin-glass state exists (at least at finite temperature) in two dimensions. A diversity of approaches has been used to study the system, but it is still not fully understood.

Most of the early Monte Carlo work[1,2] predicted a transition from ferromagnetic to spin-glass ordering for $p$ near to 0.1. It has been argued[3] that computer experiments model a nonequilibrium situation, and more recent Monte Carlo calculations,[4] which attempt to overcome this criticism, indicate that a spin-glass phase exists only at $T=0$.

There is disagreement between different real-space renormalization-group results. Jayaprakash *et al.*,[5] for example, predict a transition to a spin-glass state, while the work of Southern *et al.*[6] indicates that it is a paramagnetic state that occurs. There is also dispute over the lower critical dimensionality $d_c$ of a spin-glass. It is, however, quite possible[7,8] that $d_c \simeq 2$.

Since the work of Toulouse,[9] the concept of frustration has been emphasized in discussions of the random-bond system. This is the disorder associated with plaquettes rather than bonds that cannot be eliminated by gauge transformations. Studies which explore particularly the gauge-invariant aspects of the problem have been made by Fradkin *et al.*,[10] Kogut,[11] and Schuster.[12]

There have been various attempts[1,13–15] to construct (essentially by hand) ground states of the system, and to investigate the spatial extent of "packets of solidary spins" as a function of the concentration of frustrated plaquettes. In the references cited, the existence of a spin-glass ground state was inferred, because a proportion of the spins are locked in a fixed relative orientation over the whole area of the sample studied. In analogous work on the diluted triangular antiferromagnet, Blackman *et al.*[16] also find an extensive region of locked together spins, but employ evidence from a real-space renormalization-group calculation to conclude that the packets of solidary spins have a large but not infinite extent.

Mention should also be made of calculations[17–20] on inhomogeneous but exactly soluble models. Some useful results emerge including the suggestion[20] that fully frustrated systems form a universality class.

In the present paper, we investigate what contribution the combinatorial or Pfaffian method[21,22] can make to the understanding of the frustration problem. This was one of the earliest approaches to the pure two-dimensional (2D) Ising model, but the formalism is also valid for the disordered system. In this method the zero-field thermodynamics are related to the behavior of the determinant of a skew symmetric matrix. It is trivial to relate this matrix to one that is Hermitian and, since the problem is then expressed in terms of a matrix with real eigenvalues, an analogy exists with models of excitations in disordered systems (e.g., electronic tight-binding alloy models). It is possible that some of the methodology developed for excitation problems could be useful in the present context. Although relating the disordered Ising model to the random-alloy problem is not new, the connection has not been made previously in the way described here. In particular the manner in which frustration manifests itself in the present formalism is particularly interesting.

In Sec. II, we give a brief summary of the combinatorial method and its reexpression in terms of Hermitian matrices. The features of the eigenvalue spectrum that are important in determining such quantities as the specific-heat and pair-correlation function are investigated. The frustration aspects of the problem are pursued in Sec. III. It is shown that there is a one-to-one correspondence between frustrated plaquettes and localized eigenvalues which appear within a band gap as a consequence of the presence of frustration. The number of local modes and the temperature dependence of their eigenvalue near $T=0$ are gauge-invariant quantities. Isolated defects and also small groups of defects are studied with regard to their local-mode behavior. In Sec. IV higher concentrations of defects are examined numerically to investigate impurity-band formation. The purpose of the paper is to describe the formalism and to show that certain features of the local modes make them a more attractive entity than the frustrated plaquettes with which to study the 2D Ising system.

## II. FORMALISM

The partition function for the nearest-neighbor Ising model on an $N$-site square lattice is

$$Z=\left[\prod_{\langle ij\rangle}\cosh K_{ij}\right]\left[\mathrm{Tr}\prod_{\langle ij\rangle}(1+t_{ij}S_iS_j)\right] . \tag{2.1}$$

$K_{ij}(=J_{ij}/kT)$ is the coupling between spins and $t_{ij}=\tanh K_{ij}$. The trace is over the $2^N$ spin configurations ($S_i=\pm 1$) and the products are over the $2N$ pairs of nearest-neighbor sites $\langle ij\rangle$. In the Pfaffian method,[22] the second factor in (2.1) can be written diagrammatically as a sum over closed polygons. Green and Hurst[22] showed how this sum can be expressed as a determinant so that

$$\ln Z=\sum_{\langle ij\rangle}\ln\cosh K_{ij}+N\ln 2+\tfrac{1}{2}\ln|D| . \tag{2.2}$$

$|D|$ is a $4N\times 4N$ skew symmetric determinant sparsely filled with $4\times 4$ blocks which either are associated with a particular lattice site or connect pairs of sites.

Following Green and Hurst[22] it is convenient to associate a group of four points with each site on the square lattice as in Fig. 1. $D$ then comprises diagonal blocks $U$ given by

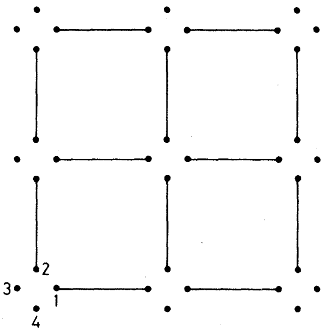

FIG. 1. Section of lattice showing group of four points associated with each site. Labeling of points displayed at one of the sites.

$$U=\begin{bmatrix}0&1&-1&1\\-1&0&1&-1\\1&-1&0&1\\-1&1&-1&0\end{bmatrix} . \tag{2.3}$$

$U$ connects the four points within the group, labeling being counterclockwise as shown in Fig. 1. The off-diagonal block of $D$ connecting the group of points associated with site $i$ to the neighboring group along the positive Cartesian $x$ axis at $j$ is $-X$, where

$$X=\begin{bmatrix}0&0&t_{ij}&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{bmatrix} . \tag{2.4}$$

Similarly if $j$ is the nearest neighbor in the positive $y$ direction, then the off-diagonal block is $-Y$, where

$$Y=\begin{bmatrix}0&0&0&0\\0&0&0&t_{ij}\\0&0&0&0\\0&0&0&0\end{bmatrix} . \tag{2.5}$$

If $j$ is a neighbor in a negative direction the appropriate blocks are $+\tilde{X}$ and $+\tilde{Y}$, where tildes represent transposes. Although the formalism was originally presented for a perfect lattice, it is also valid for any distribution of values of $J_{ij}$. Villain,[17] for example, has used the method in his fully frustrated model.

There is some desirability in working with Hermitian matrices, if for no other reason than the possibility of developing correspondences with the problem of single particle excitations in alloys. This is easily accomplished by multiplying each element of $D$ by $i$. Clearly $|D|$ is unchanged: It is merely multiplied by unity ($i^{4N}$). We now replace Eqs. (2.3)–(2.5) by

$$U=\begin{bmatrix} 0 & i & -i & i \\ -i & 0 & i & -i \\ i & -i & 0 & i \\ -i & i & -i & 0 \end{bmatrix},$$

$$X=\begin{bmatrix} 0 & 0 & it_{ij} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \tag{2.6}$$

$$Y=\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & it_{ij} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

With these definitions, Eq. (2.2) is unchanged but $D$ is Hermitian. The eigenvalue spectrum is now real and symmetric about zero (all odd moments of $D$ vanish).

In some contexts (e.g., numerical calculation) it may be more convenient to manipulate real symmetric matrices. This can be achieved by working with the square of $D$ ($H=D^2$), when (2.2) is replaced by

$$\ln Z=\sum_{\langle ij\rangle} \ln\cosh K_{ij}+N\ln 2+\tfrac{1}{4}\ln|H| . \tag{2.7}$$

$H$ has the same block pattern as $D$ and is real and symmetric. The blocks are less sparse than those appearing in $D$, however. $H$ is positive semidefinite and all its eigenvalues are doubly degenerate.

In terms of the eigenvalues $\epsilon_\lambda$ of $D$, we can write

$$\ln|D|=2\sum_{\lambda}\ln\epsilon_\lambda , \tag{2.8}$$

where the sum is over the positive eigenvalues. It is then straightforward to write (2.2) in terms of a density of states $\rho(\epsilon)$,

$$\ln Z=\sum_{\langle ij\rangle}\ln\cosh K_{ij}+N\ln 2 + \int \ln\epsilon\rho(\epsilon)d\epsilon . \tag{2.9}$$

The integral is over $\epsilon\geq 0$, and $\int\rho(\epsilon)d\epsilon=2N$. Equation (2.7) can be similarly written in terms of the density of states, $\rho_H(\epsilon)$, associated with $H$,

$$\ln Z=\sum_{\langle ij\rangle}\ln\cosh K_{ij}+N\ln 2 +\tfrac{1}{4}\int \ln\epsilon\rho_H(\epsilon)d\epsilon , \tag{2.10}$$

where the integrated density of states is now $\int\rho_H(\epsilon)d\epsilon=4N$. The relationship between the two densities is

$$\rho(\epsilon)=\epsilon\rho_H(\epsilon^2) . \tag{2.11}$$

It is straightforward to show for a perfect system ($J_{ij}=J=\text{const}$) that $\rho_H(\epsilon)$ has the step-function discontinuity, $\Theta(\epsilon-\epsilon_0)$ at the lower band edge, $\epsilon_0$, that is typical of excitation models in two dimensions. The lower band edge has a parabolic temperature dependence near the critical temperature: $\epsilon_0\propto(T-T_c)^2$. The logarithmic divergence in the specific heat of the pure Ising system immediately follows using (2.10) and the standard relation

$$C=\beta^2 d^2\ln Z/d\beta^2 ,$$

where $\beta=1/kT$.

It is instructive to show (Fig. 2) the spectral bounds of $D$ for the perfect system obtained by the usual transformation to reciprocal space. There are two bands which broaden as temperature decreases and touch at $T=0$. The figure is reminiscent of diagrams appearing in introductory solid-state texts to illustrate the formation of energy bands from atomic energy levels as atoms are brought closer to-

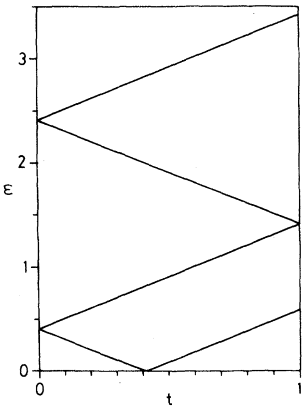

FIG. 2. Spectral bounds for perfect Ising system. Horizontal axis represents temperature variation, $t=\tanh(J/kT)$. $N$-fold–degenerate levels at $T=\infty$ are at $\epsilon=\sqrt{2}\pm 1$. Limits at $T=0$ of the upper and lower bands are, respectively, $2+\sqrt{2},\sqrt{2}$ and $\sqrt{2},2-\sqrt{2}$. Critical temperature is at $t=\sqrt{2}-1$. The gradients, $d\epsilon/dt$, of all lines are $\pm 1$.

gether. Here temperature variation replaced atomic separation. The weight of each band is $N$. The lower bound reaches zero at $T_c$. Two more bands are symmetrically placed in the negative eigenvalue region.

A further quantity one can obtain from this formalism is the spin-spin correlation function. Consider two arbitrary spins $S_1$ and $S_2$. The pair correlation function $p_{12}$ ($=\langle S_1S_2\rangle$) is given by

$$p_{12}^2=\left[\prod_{\langle ij\rangle} t_{ij}\right]^2\frac{|D^*|}{|D|}\ , \tag{2.12}$$

where $|D|$ is the determinant defined earlier. $|D^*|$ is the determinant obtained from $|D|$ by replacing the $t_{ij}$ for the bonds in an arbitrary continuous chain linking $S_1$ and $S_2$ by their reciprocals $t_{ij}^{-1}$. The prefactor in (2.12) is just the product of the $t_{ij}$ for the bonds in the chain. The equation for the correlation function originates from an expression similar to (2.1) but with the inclusion of a product of spin operators within the trace. One thus has factors like

$$S_iS_j(1+t_{ij}S_iS_j)\ .$$

Rewriting this as

$$t_{ij}(1+t_{ij}^{-1}S_iS_j)\ ,$$

the reason for the form of (2.12) becomes immediately apparent. Although the magnitude of $p_{12}$ is determined by (2.12), it is necessary to return to basic definition in terms of Pfaffians (Ref. 22) if the sign also is required.

Following a similar development to that leading to (2.9), we can rewrite (2.12) as

$$p_{12}=\left[\prod_{\langle ij\rangle} t_{ij}\right]\exp\left[\int \ln\epsilon\,\Delta\rho(\epsilon)d\epsilon\right]\ , \tag{2.13}$$

where $\Delta\rho$ is the change in density of states that occurs when the continuous chain of reciprocal defects is introduced into the system. Clearly $p_{12}$ must depend only on the positions of $S_1$ and $S_2$ and be independent of the path connecting them.

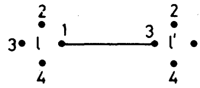

FIG. 3. A single bond defect causes a perturbation associated only with points $(l,1)$ and $(l',3)$.

Let us consider the effect of introducing a single reciprocal defect. This will determine nearest-neighbor correlations. The basis states of the defect subspace (see Fig. 3) are $|l,1\rangle$ and $|l',3\rangle$. $D^*$ is obtained from $D$ by a perturbation $V$ that, within this basis, is

$$V=\begin{bmatrix} 0 & -iv \\ iv & 0 \end{bmatrix}\ , \tag{2.14}$$

where $v=(t^{-1}-t)$ and $t=\tanh K$. The change $\Delta\rho$ in the density of states can be found by standard resolvent Green's-function techniques, where Green's functions for the unperturbed lattice are defined as follows:

$$g(\epsilon)=(\epsilon I-D)^{-1},\quad G(\epsilon^2)=(\epsilon^2 I-H)^{-1}\ . \tag{2.15}$$

Although we will not use the second form of (2.15), we note for completeness that the two are related by

$$\begin{aligned} G(\epsilon^2)&=-g(\epsilon)g(-\epsilon)\\ &=(2\epsilon)^{-1}[g(\epsilon)-g(-\epsilon)]\ . \end{aligned} \tag{2.16}$$

The Green's functions can be evaluated by transforming to reciprocal space in the usual way. The particular ones required here are, in a notation obvious from Fig. 3,

$$g_{ll}^{11}=g_{l'l'}^{33}=\pi^{-2}\int_0^\pi\int_0^\pi d\theta\,d\phi[\epsilon^3-\epsilon(3+2t\cos\theta+t^2)]/f(\epsilon;\theta,\phi)\ , \tag{2.17a}$$

$$g_{ll'}^{13}=-g_{l'l}^{31}=i\pi^{-2}\int_0^\pi\int_0^\pi d\theta\,d\phi[(3t^2-1-\epsilon^2)\cos\theta+t(t^2+1-\epsilon^2)]/f(\epsilon;\theta,\phi)\ , \tag{2.17b}$$

where

$$f(\epsilon;\theta,\phi)=P-Q(\cos\theta+\cos\phi) \tag{2.18a}$$

and

$$P=\epsilon^4-\epsilon^2(6+2t^2)+(1+t^2)^2\ , \tag{2.18b}$$

$$Q=2t(\epsilon^2+1-t^2)\ . \tag{2.18c}$$

Equations (2.17) can be simplified into the following form:

$$g_{ll}^{11}=g_{l'l'}^{33}=\epsilon tQ^{-1}(1-Ph)+\epsilon(\epsilon^2-3-t^2)h\ , \tag{2.19a}$$

$$\begin{aligned} g_{ll'}^{13}=-g_{l'l}^{31}=&\,i\tfrac{1}{2}(\epsilon^2+1-3t^2)Q^{-1}(1-Ph)\\ &+it(t^2+1-\epsilon^2)h\ , \end{aligned} \tag{2.19b}$$

where

$$h=\pi^{-2}\int_0^\pi\int_0^\pi f^{-1}d\theta\,d\phi\ . \tag{2.20}$$

$h$ can be expressed as an elliptic integral,[23]

$$h=2(\pi P)^{-1}K\left[\left[\frac{2Q}{P}\right]^2\right] . \qquad (2.21)$$

A consequence of the reciprocal defect is the appearance of a pair of local modes in the band gap at high temperatures. The local-mode condition is the usual one, $|I-gV|=0$, where $V$ is given by (2.14) and $g$ here is the Green's-function matrix in the same subspace. The local-mode condition written out fully is

$$1-iv(g_{ll'}^{13}-g_{l'l}^{31})+v^2(g_{ll'}^{13}g_{l'l}^{31}-g_{l'l'}^{33}g_{ll}^{11})=0 . \qquad (2.22)$$

This has a solution for all temperatures greater than $T_c$. The position of the local mode is plotted in Fig. 4. The second one occurs symmetrically at negative $\epsilon$.

The scattering matrix of the single bond defect is given by

$$T=V(I-gV)^{-1} , \qquad (2.23)$$

which has a pair of poles whose position is given by (2.22). The change $\Delta\rho$ in the density of states when a chain of defects is present can be written

$$\Delta\rho=gTg+gTgTg+\cdots . \qquad (2.24)$$

There is a restricted summation in the nested $g$'s as all scattering at a single defect has been included in (2.23). $\Delta\rho$ corresponds to the spectrum produced by a linear chain of atoms with two energy levels per site which are broadened by a long-range overlap (the nested $g$'s). As the length of the chain approaches infinity a finite density of states is produced at $\epsilon=0$ which, from (2.13), causes $p_{12}\rightarrow 0$.

The actual calculations of the pair correlation is facilitated if (2.13) is rewritten in a different form. For a single reciprocal defect the subspace comprises two basis states (Fig. 3). If the spins $S_1$ and $S_2$ are separated by $n$ bonds, then the corresponding subspace is of size $2n$. Let us denote the perturbation and the associated scattering matrix by $V^{(n)}$ and $T^{(n)}$, where

$$T^{(n)}=V^{(n)}(I-gV^{(n)})^{-1} .$$

The change in density of states relevant to (2.13) is

$$\Delta\rho=-\pi^{-1}\mathrm{Im}\,\mathrm{Tr}(gT^{(n)}g) ,$$

which can be expressed in the usual way[24] as

$$\Delta\rho=-\frac{1}{\pi}\mathrm{Im}\frac{d}{d\epsilon}\ln|I-gV^{(n)}| . \qquad (2.25)$$

A useful relation for an arbitrary function $F(\epsilon)$, which is analytic everywhere except for a cut along the real axis, is

$$\int_0^\infty \ln\epsilon\,\mathrm{Im}\frac{d}{d\epsilon}F(\epsilon)d\epsilon=\frac{\pi}{2}F(0) . \qquad (2.26)$$

This is easily obtained from the Kramers-Kronig relations with the condition on the function that $\mathrm{Im}F(\epsilon)\ln\epsilon\rightarrow 0$ as $\epsilon\rightarrow 0$. From (2.25) and (2.26) the exponent of (2.13) is rewritten as $\frac{1}{2}\ln|I-gV^{(n)}|_0$, where the subscript indicates evaluation at $\epsilon=0$. Thus,

$$p_{12}=\left[\prod_{\langle ij\rangle}t_{ij}\right]|I-gV^{(n)}|_0^{1/2} . \qquad (2.27)$$

If $g$ is the Green's function of the perfect lattice and $S_1$ and $S_2$ are widely separated, the determinant in (2.27) can be evaluated by the Kac-Szegö theorem.[25]

It is instructive to use (2.27) to retrieve the familiar expressions for the nearest-neighbor correlation functions. The determinant is now the left-hand side of (2.22) evaluated at $\epsilon=0$. From (2.19), this can be simplified to $(1-ivg_{ll'}^{13})^2$, and, denoting $-ig_{ll'}^{13}$ by $h_{13}$, we obtain for neighboring spins,

$$\langle S_1S_2\rangle=\tanh K+h_{13}\mathrm{sech}^2K . \qquad (2.28)$$

$h_{13}$ is related to the function $I$, defined in Eq. (177) of Domb's review.[26] In particular, at $T_c$, $h_{13}=(2\sqrt{2})^{-1}$, and so $\langle S_1S_2\rangle=2^{-1/2}$.

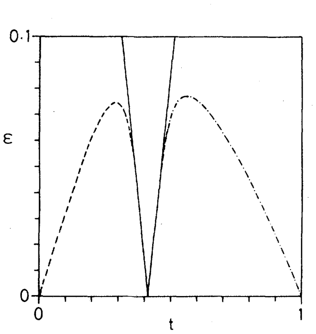

FIG. 4. Lower bound to eigenvalue spectrum for pure system (solid line). Position of local mode for reciprocal defect (dashed line). Position of local mode for negative defect (dashed-dotted line)—this case is discussed in Sec. III.

## III. FRUSTRATION

We consider how the eigenvalue spectrum is changed when a single antiferromagnetic bond replaces one of the ferromagnetic ones ($J\rightarrow -J$). Like the reciprocal defect in the preceding section, the negative bond also produces a local mode but, in this case, in the low-temperature region ($T < T_c$). We can again use (2.22) to determine the local-mode position; $v$ is now equal to $-2t$. The position of the local mode and its variation with temperature is shown in Fig. 4. By expanding the quantities appearing in (2.22) in terms of $\exp(-2J/kT)$, it is easily shown that the local-mode eigenvalue approaches zero as $T \to 0$ like $\exp(-2J/kT)$.

The necessity for the existence of the local mode is immediately appreciated from a consideration of the zero-temperature free energy. The first term of Eq. (2.9) gives a contribution $-2NJ$ to the free energy (there are $2N$ bonds). As a result of the "wrong bond" that occurs in the single-defect system the actual free energy is

$$F = -2NJ + 2J . \tag{3.1}$$

It is the local mode and its exponential temperature dependence that gives the correction $2J$ through the third term of (2.9).

We turn now to the more general case in which one bond of the lattice, all of whose bonds have value $J$, is replaced by one of value $-J'$. Again, expanding the functions appearing (2.22) in powers of small quantities, the temperature dependence of the local mode can be obtained. The result is

$$\epsilon = \pm \frac{1}{2} \left[ \exp\left[\frac{-2J'}{kT}\right] + 5 \exp\left[\frac{-6J}{kT}\right] \right] . \tag{3.2}$$

Which term of (3.2) is dominant depends on whether $J' \lessgtr 3J$. If $J' < 3J$, the antiferromagnetic bond is the wrong bond in the ground state. If $J' > 3J$, a configuration of lower energy can be found. The two cases are illustrated in Fig. 5. Clearly the correct zero-temperature free energy is given by (2.9) and (3.2). For the rest of this paper we restrict ourselves to $J' = J$.

These singularities in the band gap are highly localized spatially. At $T = 0$, we have a doubly degenerate local mode at $\epsilon = 0$, whose eigenfunctions can be written in an obvious notation (see Fig. 6),

$$|\alpha\rangle = 8^{-1/2}(\,|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle - |7\rangle + |9\rangle + |10\rangle\,) , \tag{3.3a}$$

$$|\beta\rangle = 8^{-1/2}(\,|5\rangle + |6\rangle - |8\rangle - |9\rangle + |11\rangle - |12\rangle - |13\rangle - |14\rangle\,) . \tag{3.3b}$$

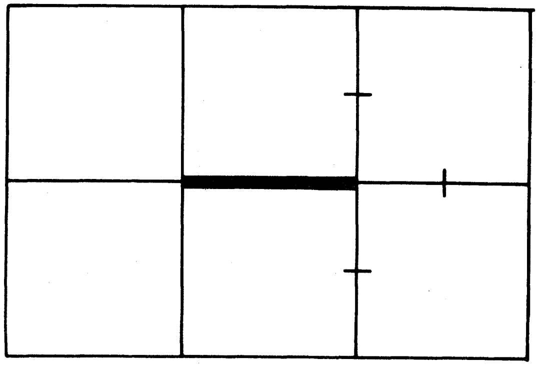

FIG. 5. A single negative defect denoted by the heavy line. If $J' < 3J$, it is also the wrong bond in the ground state. If $J' > 3J$ a state of lower energy exists, for example, that in which slashed lines denote wrong bonds.

Note that the eigenfunctions are localized on the perimeter of the frustrated plaquettes for this degenerate $\epsilon = 0$ pair. The correct linear combination to use as we move slightly away from zero temperature is

$$2^{-1/2}(\,|\alpha\rangle \pm i\,|\beta\rangle\,) .$$

Using this linear combination one obtains eigenvalues

$$\epsilon = \pm \tfrac{1}{2} \exp(-2J/kT)$$

by first-order perturbation theory.

Various effects arising from groupings of negative bonds can be illustrated by means of Fig. 7. The number of local-mode pairs for each configuration is given in Table I, together with the temperature dependence

$$\epsilon \propto \pm \exp(-2rJ/kT)$$

of each. Thus entry (e) indicates the presence of

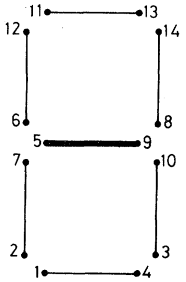

FIG. 6. Pair of frustrated plaquettes produced by single negative bond (heavy line). Figures refer to labeling of basis states which contribute to local-mode eigenfunctions.

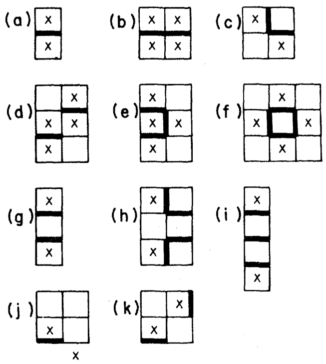

FIG. 7. Some configurations of small groups of negative bonds (heavy lines). Crosses signify frustrated plaquettes.

two local-mode pairs, one varying like $\pm\exp(-4J/kT)$ and the other like $\pm\exp(-2J/kT)$. Note that, as far as (2.9) is concerned, only one member of the pair is relevant.

Apart from cases where a wrong bond lies on the boundary of a finite sample, the boundary does not affect the number of local modes present or their eigenvalues or eigenvectors as $T\rightarrow 0$. Indeed whether the configurations in Figs. 7(a)–7(i) are isolated small samples or are embedded in large lattice is irrelevant for the particular considerations summarized in Table I.

Table I provides examples of two general rules. It will be noticed that the number of local-mode pairs is equal to the number of frustrated-plaquette pairs. Let $n_r$ denote the number of local-mode pairs whose temperature dependence is $\exp(-2rJ/kT)$. Then

TABLE I. Number of local-mode pairs for various configurations of negative bonds. Configuration letters refer to labeling in Fig. 7. $r$ is the integer appearing in $\exp(-2rJ/kT)$.

| Configuration | Number of local-mode pairs | $r$ |
|---|---|---|
| a | 1 | 1 |
| b | 2 | 1,1 |
| c | 1 | 2 |
| d | 2 | 1,1 |
| e | 2 | 2,1 |
| f | 2 | 2,2 |
| g | 1 | 2 |
| h | 1 | 2 |
| i | 1 | 3 |
| j | 1 | 1 |
| k | 1 | 2 |

$$\sum_r n_r = N_F \ , \tag{3.4}$$

where $N_F$ is the number of frustrated-plaquette pairs. If $N_W$ signifies the number of wrong bonds, it is clear, by generalizing the discussion leading to (3.1), that

$$\sum_r r n_r = N_W \ . \tag{3.5}$$

The rules (3.4) and (3.5) also apply for a finite sample with negative bonds lying on the boundary. Examples are (j) and (k) in Fig. 7. In (j) the outer boundary is a closed ring with one unsatisfied bond and the region exterior to the sample should be regarded as equivalent to a frustrated plaquette. We thus have one frustrated-plaquette pair and one wrong bond which leads to consistency between the entry in the table and the above rules. In case (k), the exterior is not frustrated. We have an internal frustrated plaquette pair, but two wrong bonds. Again there is consistency.

It is worth noting that a complete set of $T=0$ local-mode eigenvectors can be generated by inspection. As in the single-defect case [Eq. (3.3)] a convenient set can be defined, each member of which is associated with the perimeter of a single frustrated plaquette. The completeness follows from the one-to-one correspondence between frustrated plaquettes and local modes. The temperature dependence of the local modes, $\exp(-2rJ/kT)$ near $T=0$ can be obtained by perturbation theory. If $r=1$, first-order perturbation theory within the local-mode basis suffices. If $r\neq 1$, then a higher order is necessary involving states in the continuum.

It has been emphasized[9,10] that it is generally possible to realize a particular configuration of frustrated plaquettes with several different distributions of negative bonds. The frustrated-plaquette configuration is a property which is invariant under gauge transformations. Not surprisingly this gauge-invariant property extends to the local modes. Diagrams (g) and (h) of Fig. 7 are related to each other by a gauge transformation, and it will be noted that the corresponding entries in Table I are identical. The gauge invariance of the number of local-mode pairs and their temperature dependence near $T=0$ is a general result.

We complete this section with some observations relating to duality transformations. Because of the self-duality of the square lattice, the properties at high and low temperatures are related by such a transformation.[27,28] A coupling $K$ has a dual $K^*$, the relation between which can be expressed in various equivalent ways, for example,

$$\sinh 2K \sinh 2K^* = 1 \;, \qquad (3.6a)$$

$$\exp(2K^*) = \coth K \;. \qquad (3.6b)$$

If all the links are positive the transformation is quite straightforward. Consider now the negative links which have been introduced as defects and denote them by $K_1 = -K$. In order to satisfy (3.6b), it can be seen that $K_1^*$, the dual of $K_1$, must be written as $K_1^* = K^* + i\pi/2$ (there are equivalent statements to this in Refs. 10 and 29). As a consequence,

$$\tanh K_1^* = (\tanh K^*)^{-1} \;.$$

It is immediately apparent that the local modes associated with negative defects at $T < T_c$ are related to those due to reciprocal defects at $T > T_c$ by a duality transformation.

Useful relationships can be established by duality. If $Z^*$ is the partition function obtained from $Z$ by a duality transformation, then

$$\frac{Z}{\prod(\cosh 2K)^{1/2}} = \frac{Z^*}{\prod(\cosh 2K^*)^{1/2}} \;. \qquad (3.7)$$

The products are over all links $K$ and their duals $K^*$. Using (3.7) and (2.2) produces a relation between $|D|$ and its dual $|D^*|$

$$\frac{|D^*|}{|D|} = \prod_{\text{bonds}} \left[ \frac{1+t^{*2}}{1+t^2} \right] , \qquad (3.8)$$

where $t = \tanh K$ and $t^* = \tanh K^*$.

It should be emphasized that a local mode is produced not only by antiferromagnetic defects. In the case of bond dilution ($J = 0$), for example, a local mode also appears. It occurs below the band edge for $T$ just below $T_c$, and its position increases monotonically with decreasing temperature until it reaches $\epsilon \simeq 0.31$ at $T = 0$. What is characteristic of the local mode in the frustration case is its approach to zero as $T \to 0$.

## IV. FRUSTRATION AT HIGHER DENSITY

Defects, which when isolated, produce local modes, give rise to impurity bands when present in greater density. To illustrate the impurity-band formation, a numerical routine was used to obtain eigenvalues for a $10 \times 10$ sample (i.e., $4N = 400$) with a random population of defects. Because of computational advantages of real matrices, $H$ [see Eq. (2.7)] was studied rather than $D$. The results are shown in Fig. 8. The most striking feature is the recession of the host band with increasing $p$, and the eventual domination by the impurity band at low $\epsilon$. It should be noted that the width of the impurity band approaches zero in the low-temperature limit ($K \to \infty$).

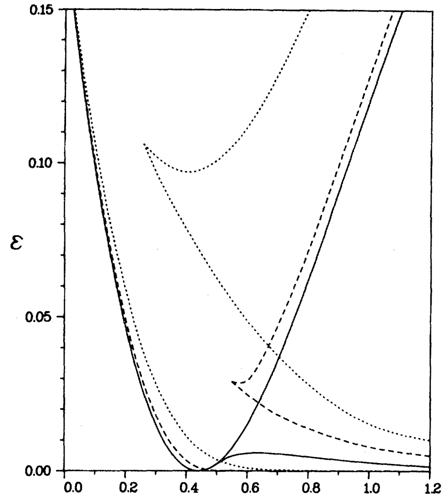

FIG. 8. Solid line represents both lower spectral bound of pure system and the single-negative-defect local-mode position. Note scales are different from those in earlier figures. $\epsilon$ refers to eigenvalues of $H$ rather than $D$ and $K = J/kT$. Lower bound of "host" band and limits of "impurity" band shown for $p = 0.05$ (dashed line) and 0.25 (dotted line).

The dominance of the impurity band can be illustrated by displaying the lower bound to the eigenvalue spectrum in greater detail. The calculation was done for samples of various size. The results

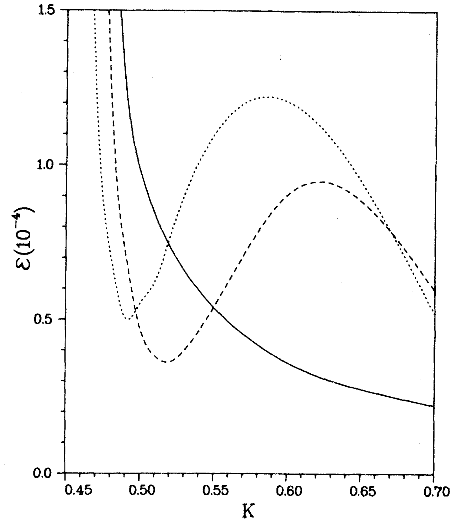

FIG. 9. Lower spectral bounds of $H$ for large sample. Solid line: $p = 0.05$; dashed: $p = 0.04$; dotted: $p = 0.03$.

for the largest sample are shown in Fig. 9. The sample size was $50\times 50$ and the method used was a block Lanczos routine developed by Scott[30] for sparse symmetric real matrices. The minimum in the spectrum, which is a feature of the host band, disappears at between 4% and 5% of defects. The value of $\epsilon$ at the lower bound is dependent on sample size. The presence or absence of a minimum at a particular $p$ is independent of the size of the sample, however.

There appears to be some sort of crossover from host-band-dominated to impurity-band-dominated behavior at about 4.5% of antiferromagnetic defects. This observation is consistent with certain aspects of the Monte Carlo calculations of Morgenstern and Binder.[4] They found a well-defined specific-heat maximum coinciding with the transition temperature for values of $p$ below about 5%. Above 5% a broader maximum was obtained, but it was not one that coincided with the transition temperature.

Clearly, to explore these matters further with the use of the present approach, one needs to study the density of states. Consideration should be given to band-tailing effects. These would be important, for example, in the rounding of the logarithmic specific-heat singularity as frustration is introduced into the system.

## V. CONCLUSIONS

The purpose of this paper has been to explore a formalism that relates the disordered 2D Ising system to the random-alloy problem in what is probably a more explicit way than has been done previously. A very instructive result of the approach is the mapping of frustrated plaquettes onto local modes. These have a characteristic behavior in the low-temperature limit that reflects the correction to be made to the internal energy because of the presence of wrong bonds. Questions of gauge invariance and duality have been considered. Apart from any insight it might provide, there are certain advantages in the present approach in comparison with those which study the frustrated plaquettes directly. For example, temperature is included in the specification of the local mode itself. Furthermore, no difficulty arises if the bonds within a plaquette differ in their magnitudes; again the local modes can encompass this subtlety.

We also considered higher concentrations of defects at which impurity-band formation becomes apparent. Using a somewhat arbitrary, but nevertheless reasonable criterion, we estimated that there is a transition from host-band- to impurity-band-dominated behavior at about 5% impurities. Consideration of various ramifications of this formalism are currently in progress.

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