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Bounded and inhomogeneous Ising models. III. Regularly spaced point defects

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We calculate exactly the transition temperature for a rectangular lattice Ising model with various types of point defects (including missing sites or vacancies) regularly distributed through the lattice on an $m \times n$ grid. We prove that for concentration $x = 1/mn$, the transition temperature is shifted to $T_c(x) = T_c(0)[1 - Q_1 x + Q_2 x^2 \ln x - Q_3 x^2 - Q_4 x^3 \ln^2 x + \ldots]$, where the constants Q_1, Q_2, Q_4, and the function $Q_3(n/m)$ are explicitly derived. The incremental free energies per isolated defect are also calculated. The various amplitudes obtained obey appropriate scaling relations.

I. INTRODUCTION

The critical behavior of magnetic systems with defects and impurities has interested many authors (see, e.g., Refs. 1–8). However, most previous studies entail approximations of various sorts whose validity is hard to establish. In particular, there are essentially no exact results available concerning the effects of a finite density of point defects on the critical behavior. In this paper, we consider an infinite rectangular Ising lattice with defects regularly distributed through the lattice on a $m \times n$ grid as illustrated in Fig. 1, and discuss the critical region by exact analysis.

When the system is dilute [i.e., $n, m \gg \xi(T)$, where $\xi(T)$ is the bulk correlation length measured in units of a lattice spacing] we find[9] that the specific heat can be expressed as a sum of the bulk specific heat $C^0(T)$ and the incremental specific heat $C^1(T)$ due to a single defect, in the form

$$C(T, m, n) = C^0(T) + (nm)^{-1} C^1(T) + O(e^{-\sigma m/\xi}, e^{-\sigma n/\xi}), \tag{1.1}$$

where $\sigma = 2$ for $T > T_c$ but $\sigma = 1$ for $T < T_c$. The bulk specific heat, as found by Onsager,[10] diverges at the bulk critical temperature T_c^0 according to

$$C^0(T)/k_B \approx -A_0 \ln|T/T_c^0 - 1| + B_0 + \cdots, \tag{1.2}$$

while the specific heat $C^1(T)$ is equal to that due to a single isolated defect[11,12] which varies as

$$C^1(T)/k_B \approx -C_0/[(T/T_c^0) - 1] - C_1[\ln|T/T_c^0 - 1|]^2 - C_2 \ln|T/T_c^0 - 1| - C_3 + \cdots. \tag{1.3}$$

When n and m are finite, we find for the various types of defects shown in Fig. 2 that the critical temperature for defect concentration $x = 1/nm$ is shifted to

$$T_c(x; \tau) = T_c^0[1 - Q_1 x - Q_2 x^2 \ln x^{-1} - Q_3(\tau) x^2 - Q_4 x^3 \ln^2 x + O(x^3 \ln x)], \tag{1.4}$$

where $\tau = n/m$. The amplitudes Q_1, Q_2, and Q_4 are found explicitly for the general ratio J_1/J_2 of horizontal to vertical interaction strengths, and are seen to satisfy the relations

$$C_0 = A_0 Q_1 \quad \text{and} \quad C_1 Q_1 = 2 A_0 Q_2. \tag{1.5}$$

These relations have been shown[13] to follow from a suitable scaling hypothesis. The function $Q_3(\tau)$, which is also calculated exactly, depends upon $\tau = n/m$, which specifies the "shape" of the defect distribution. Moreover, we show that the specific heat for a system with a finite concentration of defects still diverges logarithmically as it does in the perfect lattice; explicitly we find

$$C(n, m, T)/k_B \approx -\mathring{A}(x) \ln|\{T - T_c(x; \tau)\}/T_c^0|. \tag{1.6}$$

However, the amplitude $\mathring{A}(x)$ is calculated explicitly [for defect types (b) and (c)] in a following paper.[14] The behavior of $\mathring{A}(x)$ as $x \to 0$ again verifies the scaling hypothesis.[13] In the present paper we calculate in Sec. II, the partition function for the defects illustrated in Fig. 2. The results [for defect types (*a*) and (*c*)] are brought into tractable form using determinantal manipulations presented in Appendix A. The incremental free energy and specific heat due to a single hole (missing sites) and the corresponding shift in the critical temperature as $x \to 0$ are evaluated in Sec. III. Some of the crucial but rather tricky asymptotic analysis of double sums over lattice Green's functions is relegated to Appendix B. Using the results obtained in Sec. III, we study the incremental specific heat and temperature shifts for small x for other defects in Sec. IV. Finally, we summarize our results and compare them briefly with other work in Sec. V.

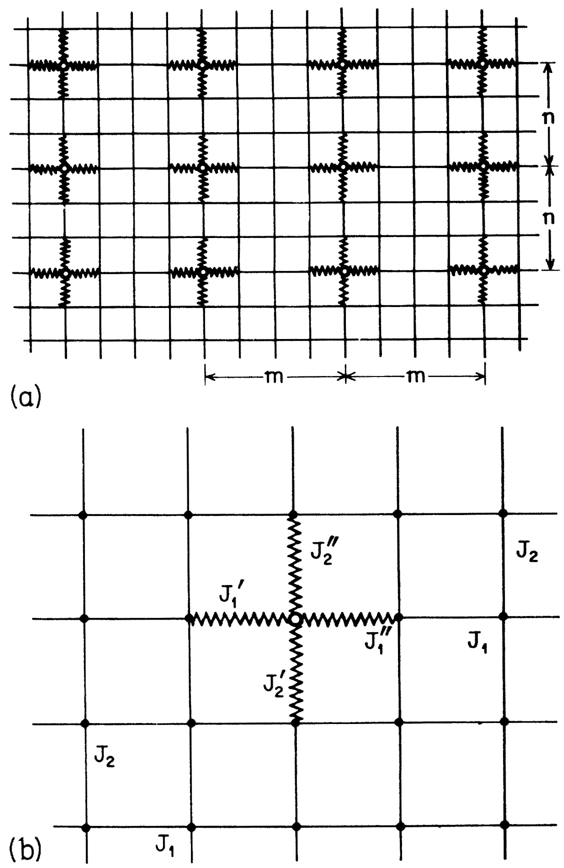

FIG. 1. (a) Rectangular Ising lattice with point defects on an $m \times n$ grid; (b) single-point defect showing modified interaction bonds.

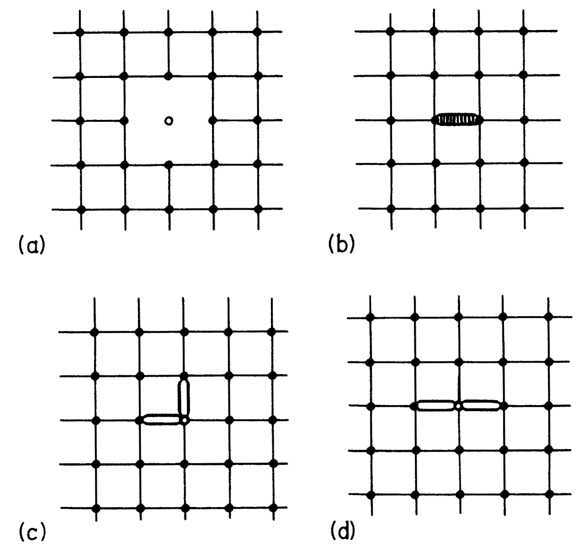

FIG. 2. Four types of point defects considered explicitly: (a) hole or vacancy, (b) single (horizontal) bond, (c) bent double bond, (d) straight double bond.

II. EVALUATION OF THE PARTITION FUNCTION

A. Pfaffian expression

Consider a $Mm \times Nn$ square lattice periodic strip ($Mm+1 \equiv 1$) whose horizontal interactions are $J_1 = k_B T K_1$ and whose vertical interactions are $J_2 = k_B T K_2$ with impurities on defects located at the sites (lm, kn) for $l = 1, 2, \ldots, M$ and $k = 1, 2, \ldots, N$. As illustrated in Fig. 1, the horizontal bonds between an impurity (or defect site) and its left and right neighbors are J_1' and J_1'', respectively, and the vertical bonds between the impurity with its down and up neighbors are J_2' and J_2'', respectively. In the thermodynamic limit $M, N \to \infty$, the partition function Z can be written in terms of the Pfaffian of an antisymmetric $4MNmn \times 4MNmn$ matrix $\underline{A}$, as

$$Z \approx \mathrm{Pf}[\underline{A}]\,(2\cosh K_1 \cosh K_2)^{MNmn} \times \left(\frac{\cosh K_1' \cosh K_1'' \cosh K_2' \cosh K_2''}{\cosh^2 K_1 \cosh^2 K_2}\right)^{MN} . \quad (2.1)$$

The matrix $\underline{A}$ has 4×4 diagonal blocks

$$\underline{A}(i,j;i,j) = \underline{a}_0 = [a_{0,\lambda\mu}] = \begin{array}{c} \\ R \\ L \\ U \\ D \end{array} \begin{array}{c} \begin{array}{cccc} R & L & U & D \end{array} \\ \begin{bmatrix} 0 & 1 & -1 & -1 \\ -1 & 0 & 1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & 1 & -1 & 0 \end{bmatrix} \end{array} , \quad (2.2)$$

for all i and j ($1 \leqslant i \leqslant Mm$ and $1 \leqslant j \leqslant Nn$), where $\lambda, \mu = R, L, U, D$, and close-to-diagonal blocks

$$\underline{A}(i,j;i,j+1) = -\underline{A}^T(i,j+1;i,j) = \underline{a}_1 + (\underline{a}_1' - \underline{a}_1)\delta_{i,ln}\delta_{j,km-1} + (\underline{a}_1'' - \underline{a}_1)\delta_{i,ln}\delta_{j,km}, \quad (2.3)$$

where the superscript T denotes matrix transposition, and

$$\underline{A}(i,j;+1,j) = -\underline{A}^T(i+1,j;i,j) = \underline{b} + (\underline{b}' - \underline{b})\delta_{i,ln-1}\delta_{j,km} + (\underline{b}'' - \underline{b})\delta_{i,ln}\delta_{j,km}, \quad (2.4)$$

for all i, j and all l, k, ($1 \leqslant l \leqslant N$, $1 \leqslant k \leqslant M$). These are the only nonvanishing blocks. In these expressions, $\underline{a}_1$ and $\underline{b}$ are 4×4 matrices, each of which has only a single nonvanishing element, namely,

$$(\underline{a}_1)_{RL} = z_1,\ (\underline{a}_1')_{RL} = z_1',\ (\underline{a}_1'')_{RL} = z_1'', \quad (2.5)$$

$$(\underline{b})_{UD} = z_2,\ (\underline{b}')_{UD} = z_2',\ (\underline{b}'')_{UD} = z_2'', \quad (2.6)$$

where the interactions enter through

$$z_i = \tanh K_i,\ z_i' = \tanh K_i',\ z_i'' = \tanh K_i'' . \quad (2.7)$$

It is obvious that the matrix elements of $\underline{A}$ form a doubly periodic set satisfying

$$\underline{A}(i,j;k,l)=\underline{A}(i+n,j;k+n,l)=\underline{A}(i,j+m;k,l+m). \tag{2.8}$$

This shows that the matrix $\underline{A}$ has a close-to-cyclic structure consisting of nearly cyclic block matrices of the size $4mn\times 4mn$. Consequently, in the thermodynamic limit the reduced free energy of the lattice with defects is

$$f(T)=\lim_{M,N\to\infty}\frac{1}{MNmn}\ln Z=\ln(2\cosh K_1\cosh K_2)+\frac{1}{2nm}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln \mathrm{Det}U(\theta_1,\theta_2)$$
$$+(nm)^{-1}\ln\left(\frac{\cosh K_1'\cosh K_2'\cosh K_1''\cosh K_2''}{\cosh^2 K_1\cosh^2 K_2}\right), \tag{2.9}$$

where $\underline{U}(\theta_1,\theta_2)$ is the $4mn\times 4mn$ matrix

$$\underline{U}(\theta_1,\theta_2)=\begin{bmatrix} \underline{B}_0 & \underline{B}_1 & & & & -\underline{B}_1''^{T}e^{-i\theta_2}\\ -\underline{B}_1^T & \underline{B}_0 & \underline{B}_1 & & & \\ & -\underline{B}_1^T & \underline{B}_0 & & & \\ & & \cdot & & & \\ & & \cdot & & & \\ & & \cdot & & & \\ & & \underline{B}_0 & & & \underline{B}_1' \\ \underline{B}_1''e^{i\theta_2} & & & & -\underline{B}_1'^{T} & \underline{B}_0' \end{bmatrix}_{n\times n}, \tag{2.10}$$

while B_0 is the $4m\times 4m$ close-to-cyclic matrix

$$\underline{B}_0=\begin{bmatrix} \underline{a}_0 & \underline{a}_1 & & & & -\underline{a}_1^{T}e^{-i\theta_1}\\ -\underline{a}_1^T & \underline{a}_0 & \underline{a}_1 & & & \\ & -\underline{a}_1^T & \underline{a}_0 & & & \\ & & \cdot & & & \\ & & \cdot & & & \\ & & \cdot & & & \\ & & \underline{a}_0 & & & \underline{a}_1 \\ \underline{a}_1e^{i\theta_1} & & & & -\underline{a}_1^{T} & \underline{a}_0 \end{bmatrix}_{m\times m}. \tag{2.11}$$

The elements of $\underline{B}_0'$ are identical to that of $\underline{B}_0$, except for those on the last row and last column, so that

$$(B_0')_{m1}e^{-i\theta_1}=-(B_0')^T_{1m}e^{i\theta_1}=\underline{a}_1'',$$
$$(B_0')_{m-1,m}=-(B_0')^T_{m,m-1}=\underline{a}_1', \tag{2.12}$$

and

$$(B_0')_{l,k}=(B_0)_{l,k}\quad\text{otherwise}. \tag{2.13}$$

Finally, the $4m\times 4m$ matrices B_1, B_1', and B_1'' are diagonal, with diagonal blocks

$$(B_1)_{ll}=(B_1)_{mm}=(B_1')_{ll}=(B_1'')_{ll}=\underline{b},\ \text{for}\ 1\le l\le m-1, \tag{2.14}$$

and

$$(B_1')_{mm}=\underline{b}',\ (B_1'')_{mm}=\underline{b}''. \tag{2.15}$$

B. Nature of the transition

We note at this point that the basic 4×4 matrices $\underline{a}_0$, $\underline{a}$, and $\underline{b}$, and hence the $4m\times 4m$ matrices $\underline{B}_0$, $\underline{B}_1$, $\underline{B}_0'$, etc., are analytic functions of z_1, z_2, etc. and hence of the temperature T. It follows that $\mathrm{Det}\underline{U}(\theta_1,\theta_2)$, which appears in (2.9) in the integrand giving the free energy, is an analytic function of T, and indeed it is also analytic in $\cos\theta_1$ and $\cos\theta_2$. From this we conclude, as in the case of the perfect Ising lattice, that the only singularity of the free energy can occur at a temperature T_0 at which the determinant of $\underline{U}(\theta_1,\theta_2)$ vanishes. It is a reflection of the translational invariance of the lattice with regularly spaced defects (as of the perfect lattice) that the determinant can vanish only for $\theta_1=\theta_2=0$. In the vicinity of such a temperature, the determinant must vary simply as $[p_0(T-T_0)^2+p_1\theta_1^2+p_2\theta_2^2]$ for small θ_1 and small θ_2. From this it follows by standard arguments that the specific heat has a singularity of the form $\dot{A}\ln|T-T_0|$, so that T_0 is evidently the critical temperature; furthermore, the specific-heat anomaly has the same singular character in the lattice with regularly spaced defects as it does in the perfect lattice. None of this, of course, is surprising, but it is worth stressing since it is widely presumed that in the case of *randomly* distributed point defects the nature of the specific-heat singularity will be very significantly different. [In principle one could ask whether there might be more than one critical temperature; in some Ising models this is certainly possible, but for the present class of defect models it is clear physically that there will be only a single critical point. For small fixed m and n, this can be checked by explicit calculation. For large m and n we will also find a single (shifted) critical point. However, we have not examined the general question more rigorously.]

Although the nature of the specific-heat singularity is unchanged, its location, $T_0=T_c(x)$, depends on the defect concentration $x=1/mn$ and so does its amplitude $\dot{A}(x)$. In the remainder of this paper we will calculate the variation of $T_c(x)$ for small x correct to order $x^3\ln^2 x$, for various types of defect. A following paper will address the question of the variation of the amplitude $\dot{A}(x)$.

C. Perfect lattice

For the perfect Ising lattice (with no defects), we have $\underline{a}_1'=\underline{a}_1''=\underline{a}_1$, $\underline{b}'=\underline{b}''=\underline{b}$; hence the corresponding matrix $\underline{U}(\theta_1,\theta_2)$ becomes

$$\underline{U}(\theta_1,\theta_2)=\begin{bmatrix} \underline{B}_0 & \underline{B}_1 & & & -\underline{B}_1^T e^{-i\theta_1} \\ -\underline{B}_1^T & \underline{B}_0 & \underline{B}_1 & & \\ & -\underline{B}_1^T & \underline{B}_0 & & \\ & & \cdot & & \\ & & \cdot & & \\ & & \cdot & & \\ & & \underline{B}_0 & & \underline{B}_1 \\ \underline{B}_1 e^{i\theta_1} & & & -\underline{B}_1^T & \underline{B}_0 \end{bmatrix}_{n\times n}, \tag{2.16}$$

which is also nearly cyclic. From this observation, we obtain

$$\mathrm{Det}\underline{U}(\theta_1,\theta_2)=\prod_{\phi_1}\prod_{\phi_2}\mathrm{Det}(\underline{a}_0+\underline{a}_1e^{i\phi_1}-\underline{a}_1^Te^{-i\phi_1}+\underline{b}e^{i\phi_2}-\underline{b}^Te^{-i\phi_2})=\prod_{\phi_1}\prod_{\phi_2}\Delta(\phi_1,\phi_2), \tag{2.17}$$

where the products run over the values

$$\phi_1=(2\pi k+\theta_1)/m,\quad k=1,\ldots,m,\quad \phi_2=(2\pi l+\theta_2)/n,\quad l=1,\ldots,n. \tag{2.18}$$

Evaluation of the 4×4 determinant yields

$$\Delta(\phi_1,\phi_2)=(1+z_1^2)(1+z_2^2)-2z_1(1-z_2^2)\cos\phi_1-2z_2(1-z_1^2)\cos\phi_2. \tag{2.19}$$

It then follows from (2.1) and (2.9) that the reduced free energy for the perfect Ising system is

$$\begin{aligned} f_0(T)&=\ln(2\cosh K_1\cosh K_2)+\frac{1}{2mn}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln\mathrm{Det}\underline{U}_0(\theta_1,\theta_2)\\ &=\ln(2\cosh K_1\cosh K_2)+\frac{1}{2}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln\Delta(\theta_1,\theta_2), \end{aligned} \tag{2.20}$$

as found and analyzed[10] in detail by Onsager.

D. Green's-function transformation

We will now transform the expression (2.9) for the free energy to a more convenient form by writing

$$\mathrm{Det}\underline{U}(\theta_1,\theta_2)=\mathrm{Det}[\underline{U}_0]\mathrm{Det}[\underline{I}+\underline{U}_0^{-1}(\underline{U}-\underline{U}_0)]=\mathrm{Det}[\underline{U}_0]\,\mathrm{Det}[\underline{\tilde{I}}+\underline{G}(\theta_1,\theta_2)\underline{y}(\theta_1,\theta_2)], \tag{2.21}$$

where $\underline{y}$ is the square submatrix of the difference matrix $\Delta\underline{U}=\underline{U}-\underline{U}_0$, which consists only of the nonvanishing rows and columns of $\Delta\underline{U}$, while $\underline{\tilde{I}}$ and the Green's-function matrix $\underline{G}$ are corresponding submatrices of $\underline{I}$ and $\underline{G}_0=\underline{U}_0^{-1}$, respectively (i.e., consisting of the same rows and columns as $\underline{y}$). On comparing (2.16) with (2.10) we find that the only nonvanishing elements of $\Delta\underline{U}=\underline{U}-\underline{U}_0$ are

$$\begin{aligned}
y_{-R,L} &= \Delta U(n,m-1,R;n,m,L) = -\Delta U(n,m,L;n,m-1,R) = -y_{L,-R} = z_1'-z_1,\\
y_{-U,D} &= \Delta U(n-1,m,U;n,m,D) = -\Delta U(n,m,D;n-1,m,U) = -y_{D,-U} = z_2'-z_2,\\
y_{R,-L} &= \Delta U(n,m,R;n,1,L) = -\Delta U^*(n,1,L;n,m,R) = -y^*_{-L,R} = (z_1''-z_1)e^{i\theta_1},\\
y_{U,-D} &= \Delta U(n,m,U;1,m,D) = -\Delta U^*(1,m,D;n,m,U) = -y^*_{-D,U} = (z_2''-z_2)e^{i\theta_2}.
\end{aligned} \tag{2.22}$$

This shows that $\underline{y}$ and $\underline{G}$ are 8×8 matrices {with rows and columns labeled $[-R, L, -U, D, R, -L, U, -D]$ or $[(n,m-1)R, (n,m)L, (n-1,m)U, (n,m)D, (n,m)R, (n,1)L, (n,m)U, (1,m)D]$}. Since the matrix $\underline{U}_0$ is nearly cyclic, its inverse[15] is easily evaluated, and we find that it is given by the matrix elements

$$\begin{aligned}
[l,k]_{\lambda\mu} &= [U_0^{-1}]_{(i,j)\lambda;(i+l,j+k)\mu} = [U_0^{-1}]_{(0,0)\lambda;(l,k)\mu}\\
&= \frac{1}{mn}\sum_{\phi_1}\sum_{\phi_2} e^{-ik\phi_1-il\phi_2}\{\underline{A}^{-1}(\theta_1,\theta_2)\}_{\lambda\mu},
\end{aligned} \tag{2.23}$$

where ϕ_1 and ϕ_2 run over the values defined by (2.18) and where

$$\underline{A}^{-1}(\phi_1,\phi_2) = \Delta(\phi_1,\phi_2)^{-1}\begin{bmatrix} h-h^* & h+h^*-ghh^* & 2-gh^* & 2-gh\\ -h-h^*+g^*hh^* & -h+h^* & -2+g^*h^* & 2-g^*h\\ -2+g^*h & 2-gh & -g+g^* & g+g^*-gg^*h\\ -2+g^*h^* & -2+gh^* & -g-g^*+gg^*h^* & g-g^* \end{bmatrix}, \tag{2.24}$$

in which

$$g = 1+z_1e^{i\phi_1}, \quad h = 1+z_2e^{i\phi_2}, \tag{2.25}$$

while the determinant $\Delta(\phi_1,\phi_2)$ was defined in (2.19). Finally, the matrix $\underline{G}$ is an 8×8 submatrix of $\underline{G}_0=\underline{U}_0^{-1}$, whose elements are represented by $[l,k]_{\lambda\mu}$.

On substituting (2.21) into (2.9), we find that the reduced free energy for the system with defects can be expressed as

$$f(T) = f_0(T) + \frac{1}{2mn}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln\operatorname{Det}[\underline{\tilde{I}}+\underline{Gy}] + (mn)^{-1}\ln\left(\frac{\cosh K_1''\cosh K_1''\cosh K_2'\cosh K_2''}{\cosh^2 K_1\cosh^2 K_2}\right). \tag{2.26}$$

Thus the calculation of the free energy is reduced to the calculation of a double integral over a logarithm of an 8×8 determinant of elements defined in terms of double sums.

III. VACANCIES OR MISSING SITES

Consider now the case when the impurities or defects are vacancies or holes formed of four missing bonds [see Fig. 2(a)], so that $z_1'=z_1''=z_2'=z_2''=0$. The free energy of the system given by (2.26) can be rewritten as

$$f(T) = f_0(T) + \frac{1}{2mn}\ln(z_1^4z_2^4) - \frac{1}{nm}\ln(\cosh^2K_1\cosh^2K_2) + \frac{1}{2mn}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln|\underline{y}^{-1}+\underline{G}|. \tag{3.1}$$

It turns out that the determinant of the 8×8 matrix $\underline{y}^{-1}+\underline{G}$ can, in this case, be reduced to a determinant of a 4×4 matrix, namely,

$$|\underline{y}^{-1}(\theta_1,\theta_2)+\underline{G}(\theta_1,\theta_2)| = (z_1z_2)^{-4}|[0,0]_{\lambda\mu}|, \tag{3.2}$$

in which the elements $[0,0]_{\lambda\mu}$ are defined by (2.23). The derivation of this formula is presented in Appendix A.

A. Free energy due to a single hole

When $n,m\to\infty$, it is easily seen that the double sum in (2.23) becomes a double integral. If we thus define

$$A_{pq} = \int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\cos p\phi_1\cos q\phi_2\,\Delta^{-1}(\phi_1,\phi_2), \tag{3.3}$$

with $\Delta(\phi_1, \phi_2)$ given by (2.19), it is not hard to check the relations

$$[0,0]^\infty_{RR} = [0,0]^\infty_{LL} = [0,0]^\infty_{UU} = [0,0]^\infty_{DD} = 0, \tag{3.4}$$

$$[0,0]^\infty_{RL} = -[0,0]^\infty_{LR} = (1-z_2^2)A_{00} - z_1(1+z_2^2)A_{10} - 2z_1z_2A_{11}, \tag{3.5}$$

$$[0,0]^\infty_{UD} = -[0,0]^\infty_{DU} = (1-z_1^2)A_{00} - z_2(1+z_1^2)A_{01} - 2z_1z_2A_{11}, \tag{3.6}$$

where the superscript ∞ denotes the condition $n, m \to \infty$, and

$$[0,0]^\infty_{RU} = -[0,0]^\infty_{UR} = [0,0]^\infty_{RD} = -[0,0]^\infty_{DR} = -[0,0]^\infty_{LU} = [0,0]^\infty_{LD} = -[0,0]^\infty_{DL} = [0,0]^\infty_{UL} = A_{00} - z_1A_{10} - z_2A_{01} - z_1z_2A_{11}. \tag{3.7}$$

It can be seen from these equations that the matrix in (3.2) becomes antisymmetric when $n, m \to \infty$. Hence in this limit we have

$$|y^{-1}+G| = (z_1z_2)^{-4}\{[0,0]^\infty_{RL}[0,0]^\infty_{UD} - [0,0]^\infty_{RU}[0,0]^\infty_{LD} + [0,0]^\infty_{RD}[0,0]^\infty_{LU}\}^2 = (z_1z_2)^{-4}\{[0,0]^\infty_{RL}[0,0]^\infty_{UD} - 2([0,0]^\infty_{RU})^2\}. \tag{3.8}$$

Consequently the free energy of (3.1) can be written as the bulk free energy f_0 plus the free energy f_1 due to a *single* hole, namely,

$$f \approx f_0 + (nm)^{-1}f_1 + O(e^{-\sigma m/\xi_1}, e^{-\sigma n/\xi_2}), \tag{3.9}$$

where

$$f_1(T) = \ln[(1-z_1^2)(1-z_2^2)] + \ln|[0,0]^\infty_{RL}[0,0]^\infty_{UD} - 2([0,0]^\infty_{RU})^2|, \tag{3.10}$$

while ξ_1 and ξ_2 are the correlation lengths for the horizontal and vertical directions and $\sigma=2$ for $T>T_c$ but $\sigma=1$ for $T<T_c$; the correction term in (3.9) is discussed further in Appendix C.

We can calculate f_1 exactly: To simplify the notation let us put

$$a = (1+z_1^2)(1+z_2^2), \quad b = z_1(1-z_2^2), \quad c = z_2(1-z_1^2), \tag{3.11}$$

so that from (2.19) and (3.3) we have

$$A_{00} = \int_0^{2\pi} \frac{d\phi_1}{2\pi} \int_0^{2\pi} \frac{d\phi_2}{2\pi} (a - 2b\cos\phi_1 - 2c\cos\phi_2)^{-1}. \tag{3.12}$$

This integral can be evaluated in closed form as[16,17]

$$A_{00} = (2/\pi)K(\kappa)/[(t^2+4b)(t^2+4c)]^{1/2}, \tag{3.13}$$

where $K(\kappa)$ is the complete elliptic integral of the first kind and of modulus κ given by

$$\kappa^2 = 16bc/(t^2+4b)(t^2+4c), \tag{3.14}$$

where the *deviation from the critical temperature* is measured by the variable

$$t = 1 - z_1 - z_2 - z_1z_2 \approx (1+z_{1c})(1+z_{2c})\{-[(1-z_{1c})J_1 + (1-z_{2c})J_2](\beta-\beta_c) + [z_{1c}(1-z_{1c})J_1^2 + z_{2c}(1-z_{2c})J_2^2 - (1-z_{1c})(1-z_{2c})J_1J_2](\beta-\beta_c)^2\}, \tag{3.15}$$

with $\beta = 1/k_BT$. The critical temperature $T_c^0 = 1/k_B\beta_c$ of the perfect Ising lattice is determined by

$$\exp(-2J_1/k_BT_c^0) = \tanh(J_2/k_BT_c^0). \tag{3.16}$$

In the symmetric case $J_1 = J_2 = k_BTK$, we have

$$t = -4\sqrt{2}(\sqrt{2}-1)(K-K_c) + 4(\sqrt{2}-1)^3(K-K_c)^2 + O[(K-K_c)^3]. \tag{3.17}$$

It is also useful to note the easily checked relation

$$a - 2b - 2c = t^2. \tag{3.18}$$

The integral A_{10} can be evaluated exactly,[16,18] yielding

$$A_{10} = \int_0^{2\pi} \frac{d\theta_1}{2\pi} \int_0^{2\pi} \frac{d\theta_2}{2\pi} \cos\phi_1(a - 2b\cos\phi_1 - 2c\cos\phi_2)^{-1} = A_{00} - \frac{1-\Lambda_0(\theta,\kappa)}{2b}, \tag{3.19}$$

where $\Lambda_0(\theta, \kappa)$ is Heuman's lambda function[14] with modulus κ given by (3.14) and argument

$$\theta = \sin^{-1}[(t^2+4c)/(t^2+4b+4c)]^{1/2}. \tag{3.20}$$

Similarly we find

$$A_{01} = A_{00} - [1-\Lambda_0(\tilde{\theta}, \kappa)]/2c, \tag{3.21}$$

with argument now given by

$$\tilde{\theta} = \sin^{-1}[(t^2+4b)/(t^2+4b+4c)]^{1/2}. \tag{3.22}$$

Finally, the integral A_{11} can be evaluated[16,19] as

$$A_{11} = A_{00} + t^2(t^2+4b+4c)A_{00}/(8bc) - [(t^2+4b)(t^2+4c)]^{1/2}E(\kappa)/(4\pi bc), \tag{3.23}$$

where $E(\kappa)$ is the complete elliptic integral of the second kind. These results, with (3.4)–(3.7), show that all these matrix elements $[0,0]^{\infty}_{\lambda\mu}$ can be expressed in terms of elliptic integrals; the formulas are tabulated in Table I. It follows that the incremental free energy $f_1(T)$ due to a single hole can also be written in terms of elliptic integrals. In particular, in the symmetric case $J_1 = J_2 = k_B TK$, the free energy $f_1(T)$ reduces to the simple form

$$f_1(T) = \ln\{\tfrac{1}{16}(1+z^2)^2 - \tfrac{1}{2} - (1+z^2)^2E(\kappa)/4\pi - (1+z^2)\kappa' K(\kappa)/\pi + (2z^2/\pi^2\kappa^2)[E(\kappa) + 2\kappa' E(\kappa)K(\kappa) - \kappa'^3 K(\kappa)]\}, \tag{3.24}$$

in which the Heuman lambda functions cancel out, while the conjugate modulus is

$$\kappa' = (1-\kappa^2)^{1/2} = 1 - 8z^2/(1+z^2)^2, \quad z = \tanh K. \tag{3.25}$$

This result can also be obtained independently by calculating the ratio Z^h/Z, where Z^h is the partition function of a Ising system with a *single* hole present at the origin[11]; the incremental free energy may also be expressed quite simply in terms of two-spin and four-spin correlation functions of the perfect Ising lattice.[12]

In the limit $T \to T_c^0$, $(t\to 0, \kappa \to 1)$, we have[20]

$$K(\kappa) \approx \ln|4/\kappa'|, \quad E(\kappa) \approx 1 + \tfrac{1}{2}\kappa'^2 \ln|4/\kappa'|, \tag{3.26}$$

and[21]

$$\Lambda_0(\beta, \kappa) \approx 2\beta/\pi + (2/\pi)\sin\beta\cos\beta(1-\kappa)\ln|4/\kappa'|. \tag{3.27}$$

Hence the free energy $f_1(T)$ due to a single hole, in the general case, has the form

$$f_1(T) = \ln[(1-z_1^2)(1-z_2^2)] + \ln|D_0 - D_1[t\ln|t| + D_2] + D_3 t^2 \ln|t| + O(t^3\ln|t|)|, \tag{3.28}$$

as $T \to T_c$, where the amplitudes $D_i(t)$ $(i = 0, 1, 2, 3)$ are analytic functions of t, not vanishing at

TABLE I. Expressions for the matrix elements $[0,0]^{\infty}_{\lambda\mu}$.

$$b = z_1(1-z_2^2), \quad c = z_2(1-z_1^2), \quad \kappa^2 = 16bc/(t^2+4b)(t^2+4c), \quad \kappa'^2 = 1-\kappa^2,$$
$$\theta = \tan^{-1}[(t^2+4c)/4b]^{1/2}, \quad \tilde{\theta} = \tan^{-1}[(t^2+4b)/4c]^{1/2}, \quad E = E(\kappa), \quad K = K(\kappa)$$

$$[0,0]^{\infty}_{RL} = \frac{2tK\{(1+z_2) - z_1z_2t(t^2+4b+4c)/4bc\}}{\pi[(t^2+4b)(t^2+4c)]^{1/2}} + \frac{z_1z_2[(t^2+4b)(t^2+4c)]^{1/2}E}{2\pi bc} + \frac{z_1(1+z_2^2)[1-\Lambda_0(\theta,\kappa)]}{2b}$$

$$[0,0]^{\infty}_{UD} = \frac{2tK\{(1+z_1) - z_1z_2t(t^2+4b+4c)/4bc\}}{\pi[(t^2+4b)(t^2+4c)]^{1/2}} + \frac{z_1z_2[(t^2+4b)(t^2+4c)]^{1/2}E}{2\pi bc} + \frac{z_2(1+z_1^2)[1-\Lambda_0(\tilde{\theta},\kappa)]}{2c}$$

$$[0,0]^{\infty}_{RU} = \frac{2tK\{1 - z_1z_2t(t^2+4b+4c)/8bc\}}{\pi[(t^2+4b)(t^2+4c)]^{1/2}} + \frac{z_1[1-\Lambda_0(\theta,\kappa)]}{2b} + \frac{z_2[1-\Lambda_0(\tilde{\theta},\kappa)]}{2c} + \frac{z_1z_2[(t^2+4b)(t^2+4c)]^{1/2}E}{4\pi bc}$$

$t=0$ ($T=T_c^0$). They are listed in Table II.

Consequently, the incremental specific heat C_1 due to a single hole is ($\beta=1/k_BT$)

$$C^1(T)/k_B \approx \beta_c^2\,\frac{\partial^2 f_1(T)}{\partial\beta^2}$$

$$= -C_0\left[\frac{T}{T_C^0}-1\right]^{-1} - C_1\left[\ln\left|\frac{T}{T_c^0}-1\right|\right]^2 - C_2\ln\left|\frac{T}{T_c^0}-1\right| + O(1) \tag{3.29}$$

in which

$$C_0 = -\beta_c\left(\frac{\partial t}{\partial\beta}\right)_c\frac{D_{1c}}{D_{0c}},\quad C_1=C_0^2, \tag{3.30}$$

$$C_2=\beta_c^2\left(\frac{\partial^2 t}{\partial\beta^2}\right)_c\frac{D_{1c}}{D_{0c}}+2\beta_c^2\left(\frac{\partial t}{\partial\beta}\right)^2\left\{\left[\ln\left|\beta_c\left(\frac{\partial t}{\partial\beta}\right)_c\right|+D_{2c}+1\right]\frac{D_{1c}^2}{D_{0c}^2}-\frac{D_{3c}}{D_{0c}}\right\}$$

$$+2\beta_c^2\left(\frac{\partial t}{\partial\beta}\right)_c\left(\frac{\partial}{\partial\beta}\,\frac{D_1}{D_0}\right)_c, \tag{3.31}$$

where the subscript c denotes values at $T=T_c^0$.

In the symmetric case ($J_1=J_2$), we may quote the value for the incremental free energy at T_c^0,

$$f_1(T_c^0)=\ln[\sqrt{2}-1+(6-4\sqrt{2})(\pi^{-1}-\pi^{-2})]$$
$$\simeq -0.716\,0631, \tag{3.32}$$

and the values for the critical amplitudes,

$$C_0=\frac{[4-(8-4\sqrt{2})/\pi]\,\ln(\sqrt{2}+1)}{\pi[1+2(\sqrt{2}-1)(\pi^{-1}-\pi^{-2})]}$$
$$\simeq 0.773\,8464, \tag{3.33}$$

$$C_1=C_0^2\simeq 0.598\,8383,\quad C_2\simeq 0.388\,0765. \tag{3.34}$$

B. Shift in the critical temperature for finite n,m

When n and m are finite, it is clear from (3.1) that the critical temperature is determined by the condition at $\theta_1=\theta_2=0$, namely, it is a solution of

$$|\underline{y}^{-1}(0,0)+\underline{G}(0,0)|=0, \tag{3.35}$$

since, as in the perfect Ising model, this is the only possible source of a singularity in the double integral. Note, however, that this term must also cancel the singularity in $f_0(T)$ at the unshifted critical temperature of the perfect lattice. In studying this equation the main task is the analysis of the double sums

$$S_{pq}(m,n) = (nm)^{-1}\sum_{l=1}^{m}\sum_{k=1}^{n}\frac{\cos(2\pi lp/m)\cos(2\pi kq/n)}{\Delta(2\pi l/m,2\pi k/n)}. \tag{3.36}$$

Now it is easy to check from (2.23) that equations precisely similar to (3.4)–(3.7) hold for finite n and m when $\theta_1=\theta_2=0$, except that the double integrals A_{pq} are to be replaced by the double sums $S_{pq}(n,m)$. More explicitly, at $\theta_1=\theta_2=0$ we find

$$[0,0]_{RR}^0=[0,0]_{LL}^0=[0,0]_{UU}^0=[0,0]_{DD}^0=0, \tag{3.37}$$

$$[0,0]_{RL}^0=-[0,0]_{LR}^0$$
$$=(1-z_2^2)S_{00}-z_1(1+z_2^2)S_{10}-2z_1z_2S_{11}, \tag{3.38}$$

$$[0,0]_{UD}^0=-[0,0]_{DU}^0$$
$$=(1-z_1^2)S_{00}-z_2(1+z_1^2)S_{01}-2z_1z_2S_{11}, \tag{3.39}$$

where the superscript zero denotes the condition $\theta_1=\theta_2=0$, and

$$[0,0]_{RU}^0=-[0,0]_{UR}^0=[0,0]_{RD}^0=-[0,0]_{DR}^0$$
$$=-[0,0]_{LU}^0=[0,0]_{UL}^0=[0,0]_{LD}^0=-[0,0]_{DL}^0$$
$$=S_{00}-z_1S_{10}-z_2S_{01}-z_1z_2S_{11}. \tag{3.40}$$

On using the reduction formula (3.2), the critical-point equation becomes

$$|\underline{y}^{-1}(0,0)+\underline{G}(0,0)|$$
$$=\{[0,0]_{RL}^0[0,0]_{UD}^0-2([0,0]_{RU}^0)^2\}^2=0. \tag{3.41}$$

We are concerned with the study of the behavior of the critical temperature for large m and n, i.e., a low concentration of defects. Accordingly, the double sums $S_{pq}(m,n)$ must be evaluated asymptotically as $m,n\to\infty$ in the limit $t\to 0$ (i.e., $T\to T_c$). This task, which represents the hard heart of the analysis, is undertaken in Appendix

B. As might have been anticipated, the asymptotic results have, in part, a scaling form in terms of the variables $\bar{m}t$, $\bar{n}t$ and the ratio

$$\tau = \frac{\bar{n}}{\bar{m}} = \left[\frac{z_1(1-z_2^2)}{z_2(1-z_1^2)}\right]^{1/2}\frac{n}{m}, \qquad (3.42)$$

where

$$\bar{m} = m/b^{1/2} = m/[z_1(1-z_2^2)]^{1/2},$$
$$\bar{n} = n/c^{1/2} = n/[z_2(1-z_1^2)]^{1/2}. \qquad (3.43)$$

Specifically we find

$$S_{00}(m,n) = \frac{1}{t^2 mn} + \frac{1}{2\pi(bc)^{1/2}}[\ln(mn)^{1/2} + P(\bar{m}t, \bar{n}t)] + O(t^2\ln m, m^{-2}), \qquad (3.44)$$

where, with $\tau = y/x$, the scaling function is given by

$$P(x,y) = \pi|x|^{-1}(\coth\tfrac{1}{2}|y| - 2|y|^{-1} - \tfrac{1}{6}|y|) + \pi|y|^{-1}(\coth\tfrac{1}{2}|x| - 2|x|^{-1} - \tfrac{1}{6}|x|)$$
$$+ 8\pi\sum_{l=1}^{\infty}\sum_{k=1}^{\infty}[(xy + 4\pi^2\tau^{-1}l^2 + 4\pi^2\tau k^2)^{-1} - (4\pi^2\tau^{-1}l^2 + 4\pi^2\tau k^2)^{-1}]$$
$$+ \{C_E + \ln(2/\pi) - \tfrac{1}{4}\ln[(b+c)^2/bc] - \tfrac{1}{2}\ln\tau + 2F(\tau)\}, \qquad (3.45)$$

in which $C_E \simeq 0.557\,2157$ is Euler's constant, while

$$F(\tau) = \tfrac{1}{12}\pi\tau + \sum_{l=1}^{\infty}\frac{1}{l(e^{2\pi\tau l}-1)}$$
$$= -\tfrac{1}{3}\ln[\theta_2(0|i\tau)\theta_3(0|i\tau)\theta_4(0|i\tau)] + \tfrac{1}{3}\ln 2 \qquad (3.46)$$

where the $\theta_i(v|i\tau)$ are the elliptic θ functions. It is not difficult to see that $P(x,y)$ is analytic for all real x and y.

From Appendix B we obtain the further results

$$S_{10}(m,n) = S_{00}(m,n) - \frac{1}{\pi b}\tan^{-1}\left(\frac{b}{c}\right)^{1/2} + \frac{(bc)^{-1/2}}{m^2}G(\tau) + O(t^2\ln m, m^{-4}), \qquad (3.47)$$

$$S_{01}(m,n) = S_{00}(m,n) - \frac{1}{\pi c}\tan^{-1}\left(\frac{c}{b}\right)^{1/2} + \frac{(bc)^{-1/2}}{n^2}G(\tau^{-1}) + O(t^2\ln m, m^{-4}), \qquad (3.48)$$

$$S_{11}(m,n) = S_{00}(m,n) - \frac{1}{\pi(bc)^{1/2}} + \frac{(bc)^{-1/2}}{m^2}G(\tau) + \frac{(bc)^{-1/2}}{n^2}G(\tau^{-1}) + O(t^2\ln m, m^{-4}), \qquad (3.49)$$

where the function $G(\tau)$ is defined by

$$G(\tau) = \frac{\pi}{12} - \sum_{l=1}^{\infty}\frac{2\pi l}{e^{2\pi\tau l}-1} = \frac{dF}{d\tau} \qquad (3.50)$$

and hence satisfies the symmetry relation

$$G(\tau^{-1}) + \tau^2 G(\tau) = \tfrac{1}{2}\tau \qquad (3.51)$$

corresponding to interchange of m and n (or $\bar{m}$ and $\bar{n}$).

On using these asymptotic results for the $S_{pq}(m,n)$ in (3.38)–(3.40) we obtain the asymptotic forms of the matrix elements $[0,0]^0_{\lambda\mu}$. The critical-point equation, which determines the shift in critical temperature from $t=0$ to $t_c(m,n)$, then becomes

$$D_0 + 2\pi D_1(bc)^{1/2}t\,S_{00}(m,n) + E_1/mn - t^3S_{00}^2(m,n) + (E_2/mn)t\,S_{00}(m,n) \approx 0, \qquad (3.52)$$

in which $D_0(t)$ and $D_1(t)$ are given in Table II, while E_1 and E_2, which depend on m/n, are parameters listed in Table III. The neglected corrections to this equation are of orders $t^2\ln(mn)$ and $(mn)^{-2}\ln(mn)$. It is appropriate to recall at this point that $(mn)^{-1}$ is simply the *concentration, x,* of defects (holes, in this case).

Now to solve this equation we must first estimate $t_c(m,n)$ in leading order. Initially, we might suspect that t_c is of order $1/m$ (with $\tau \propto n/m$ of order unity). However, on this assumption the equation reduces to

$$D_0 + 2\pi(bc)^{1/2}D_1 t\,S_{00}(t,m,n) + O(t^2\ln mn) = 0. \qquad (3.53)$$

But when $t_c m$ is of the order of unity, it follows from (3.45) that S_{00} is also of order unity, so that the equation is, in fact, inconsistent. Thus we assume and confirm directly that t_c is of order

TABLE II. Critical amplitudes for a single defect.

$$u=\frac{4}{\pi}\tan^{-1}\left(\frac{b}{c}\right)^{1/2},\quad u'=\frac{4}{\pi}\tan^{-1}\left(\frac{c}{b}\right)^{1/2}=2-u,\quad \tilde{A}(t)=\frac{1}{2\pi(bc)^{1/2}}$$

Vacancy (a)

$$D_0(t)=\{\tfrac{1}{4}z_1(1+z_2^2)b^{-1}u+4z_1z_2\tilde{A}(t)\}\{\tfrac{1}{4}z_2(1+z_1^2)c^{-1}u'+4z_1z_2\tilde{A}(t)\}$$
$$-2\{\tfrac{1}{4}z_1b^{-1}u+\tfrac{1}{4}z_2c^{-1}u'+2z_1z_2\tilde{A}(t)\}^2$$

$$D_1(t)=\tilde{A}(t)\{(1+z_2)[\tfrac{1}{4}z_2(1+z_1^2)u'+4z_1z_2\tilde{A}(t)]+(1+z_1)[\tfrac{1}{4}z_1(1+z_2^2)b^{-1}u+4z_1z_2\tilde{A}(t)]$$
$$-4[\tfrac{1}{4}z_1b^{-1}u+\tfrac{1}{4}z_2c^{-1}u'+2z_1z_2\tilde{A}(t)]\}$$

$$D_2(t)=\tfrac{1}{2}\ln[(b+c)/64bc]$$

$$D_3(t)=2\tilde{A}(t)^2z_1z_2[z_1z_2(b+c)-bc]-\tfrac{1}{4}\tilde{A}(t)(bc)^{-1}[2z_1z_2+z_1^2(c/b)u+z_2^2(b/c)u']$$

Straight-bond defect (d)

$$\overline{D}_0(t)=\{z_1^{-1}-\tfrac{1}{4}z_1^{-1}u+\tfrac{1}{2}z_1z_2c^{-1}u'\}^2+\tfrac{1}{16}(1+z_2^2)^2b^{-2}u^2-16z_2^2\tilde{A}(t)^2$$

$$\overline{D}_1(t)=\tilde{A}(t)(1+z_2)\{2z_1^{-1}-\tfrac{1}{4}[2(1-z_2^2)-(1+z_2^2)(z_1^{-1}-z_1)]b^{-1}u+z_1z_2c^{-1}u'-4z_2(z_1^{-1}+z_1)\tilde{A}(t)\}$$

$1/mn$, i.e., proportional in leading order to the concentration x, in which case $tS_{00}(t,m,n)$ is of order unity. Accordingly, let us put

$$\tilde{A}(t)=1/2\pi(bc)^{1/2} \tag{3.54}$$

and expand $D_0(t)$ and $D_1(t)$ as

$$D_0(t)=D_{0c}+t\,D'_{0c}+O(t^2), \tag{3.55}$$

$$D_1(t)/\tilde{A}(t)=D_{1c}/\tilde{A}_c+t\,(D_1/\tilde{A})'_c+O(t^2), \tag{3.56}$$

so that (3.52) becomes

$$(t_cmn)^{-1}[D_{1c}/\tilde{A}_c+(E_2-1)/nm]+D_{0c}+[E_1+(D_1/\tilde{A})'_c]/nm$$
$$+t_c[D'_{0c}+\tfrac{1}{2}D_{1c}\ln(nm)+D_{1c}P_0(\tau)]+O(n^{-2}m^{-2}\ln n\,m)=0, \tag{3.57}$$

where $P_0(\tau)$ is the limit of $P(x,y)$ defined in (3.45) as $t=x/\overline{m}=y/\overline{n}$ approaches zero with fixed $\overline{m}$ and $\overline{n}$. We may now try a solution of the form

$$t_c(m,n)\approx -u(nm)^{-1}[1+v_1(nm)^{-1}\ln(nm)+w(nm)^{-1}+v_2(nm)^{-2}\ln^2(nm)]. \tag{3.58}$$

On substituting this trial form, dropping terms of the order $(nm)^{-2}\ln(nm)$, and comparing the remaining coefficients, we obtain, finally,

$$u=D_{1c}/\tilde{A}_cD_{0c},\quad v_1=\tfrac{1}{2}D_{1c}^2/\tilde{A}_cD_{0c}^2,\quad v_2=2v_1^2, \tag{3.59}$$

and

$$w(\tau)=(\tilde{A}_c/D_{1c})[E_2(\tau)-1]-D_{0c}^{-1}[E_1(\tau)+(D_1/\tilde{A})'_c]$$
$$+(D_{1c}/\tilde{A}_c)D'_{0c}/D_{0c}^2+(D_{1c}^2/\tilde{A}_cD_{0c}^2)P_0(\tau),\qquad \tau=\overline{n}/\overline{m}. \tag{3.60}$$

Since the variable t of (3.15) may be put in the form

$$t\approx r_1[(T/T_c^0)-1]+r_2(T/T_c^0)-1]^2, \tag{3.61}$$

where

$$r_1=T_c^0\left(\frac{\partial t}{\partial T}\right)_c=-\beta_c\left(\frac{\partial t}{\partial\beta}\right)_c,\quad r_2=\tfrac{1}{2}(T_c^0)^2\left(\frac{\partial^2t}{\partial T^2}\right)_c, \tag{3.62}$$

Eq. (3.58) for the shift in critical temperature has the alternative form

$$T_c(x)=T_c^0[1-Q_1x-Q_2x^2\ln x^{-1}-Q_3(\tau)x^2$$
$$-Q_4x^3\ln^2x+O(x^3\ln x)], \tag{3.63}$$

in which

$$Q_1=u/r_1=(r_1D_{1c}/D_{0c})/(r_1^2\tilde{A}_c), \tag{3.64}$$

$$Q_2=Q_1v_1=Q_1(r_1D_{1c}/D_{0c})^2/2(r_1^2\tilde{A}_c),$$

$$Q_4=2Q_1v_1^2, \tag{3.65}$$

TABLE III. Constants E_i.

$$\alpha=\frac{1-z_{2c}^2}{2z_{2c}},\quad \tau=\alpha\frac{n}{m},\quad u=\frac{4}{\pi}\tan^{-1}\alpha,\quad u'=2-u,$$

$$G(\tau)=\frac{\pi}{12}-\sum_{l=1}^{\infty}\frac{2\pi l}{e^{2\pi l}-1}$$

$$E_1=-[\tfrac{1}{4}(1+z_{2c}^2)(1-z_{2c}^2)^{-1}u+\pi^{-1}]\,[z_{2c}^{-1}\tau^{-1}G(\tau^{-1})+\alpha^{-1}\tau G(\tau)]$$
$$-[(1+z_{2c}^2)(8z_{2c})^{-1}u'+\pi^{-1}]\,[(1+z_{2c})(1-z_{2c})^{-1}\tau G(\tau)+\alpha\tau^{-1}G(\tau^{-1})]$$
$$+[(1-z_{2c}^2)^{-1}u+\tfrac{1}{4}(1+z_{2c})^2z_{2c}^{-1}u'+2\pi]\,2(1+z_{2c})z_{2c}^{-1}[\alpha^{-1}\tau G(\tau)+\alpha\tau^{-1}G(\tau^{-1})]$$

$$E_2=-(1+z_{2c})[z_2^{-1}\tau^{-1}G(\tau^{-1})+\alpha^{-1}\tau G(\tau)]-2(1+z_{2c})^{-1}[(1+z_{2c})(1-z_{2c})^{-1}\tau G(\tau)+\alpha\tau^{-1}G(\tau^{-1})]$$
$$+2(1+z_{2c})z_{2c}^{-1}[\alpha^{-1}\tau G(\tau)+\tau G(\tau)]$$

$$E_6=2\{z_1^{-1}-\tfrac{1}{4}z_1^{-1}u+\tfrac{1}{4}\alpha u'\}\,[(1+z_{2c})(1-z_{2c})^{-1}\tau G(\tau)-\alpha\tau^{-1}G(\tau^{-1})]$$
$$+\{-\tfrac{1}{2}(1+z_{2c}^2)^2(1-z_{2c})^{-4}\tau G(\tau)+(2/\pi)(1+z_{2c})^2(1-z_{2c})^{-2}[\alpha\tau^{-1}G(\tau^{-1})+\alpha^{-1}\tau G(\tau)]\}$$
$$-\tfrac{1}{4}(1+z_{2c}^2)(1-z_{2c})^{-2}u-(1+z_{2c})(1-z_{2c})^{-1}\pi^{-1}$$

and

$$Q_3(\tau)=Q_1[w(\tau)+u r_2/r_1^2]. \tag{3.66}$$

It can be seen from (2.20) that the specific heat for the Ising lattice without defects or impurities behaves as

$$C^0(T)\approx r_1^2\frac{\partial^2}{\partial t^2}f_0(T)$$
$$\approx r_1^2A_{00}\approx -r_1^2\tilde{A}\ln|t|, \tag{3.67}$$

where A_{00} is the double integral given by (3.12) and (3.13), and $\tilde{A}(t)$ is given by (3.54). This shows that the amplitude A_0 for the specific heat $C_0(T)$ of the perfect lattice is given by

$$A_0=r_1^2\tilde{A}_c.$$

On comparing the results for A_0, Q_1, and Q_2 with the result (3.30) for the amplitude C_0 and C_1 for the incremental specific heat due to a single hole, we find the relations

$$C_0=A_0Q_1\quad\text{and}\quad C_1Q_1=2A_0Q_2, \tag{3.68}$$

which are in precise accord with the expectations of the scaling theory.[13] In the symmetric case $J_1=J_2$, we have explicitly $K_c=\frac{1}{2}\ln(\sqrt{2}+1)$ and

$$Q_1=\frac{1-(2-\sqrt{2})/\pi}{K_c[1+2(\sqrt{2}-1)(\pi-1)/\pi^2]}\simeq 1.564\,785, \tag{3.69}$$

$$Q_2=4K_c^2Q_1^3/\pi\simeq 0.947\,401\,3,$$
$$Q_4\simeq 1.147\,211. \tag{3.70}$$

We also quote the special values

$$Q_3(1)\simeq -1.274\,047,\quad Q_3(1.5)\simeq -1.165\,338, \tag{3.71}$$
$$Q_3(2)\simeq -0.942\,1229,$$
$$Q_3(2.5)\simeq -0.657\,4839,$$
$$Q_3(3)\simeq -0.334\,6556. \tag{3.72}$$

IV. BOND DEFECTS

In this section we shall show that the incremental free energy and the shift in the critical temperature, due to other kinds of bond defects (Fig. 2), can be obtained easily by specializing the basic results of Sec. II for the general point defect shown in Fig. 1(b) with couplings J_1', J_1'', J_2', J_2''.

A. Single-bond defect (b): $J_1''=J_1$, $J_2'=J_2''=J_2$

It is obvious from (2.28) that the free energy of the system with single-horizontal-bond defects of strength J_1' is

$$f(T)=f_0(T)+(nm)^{-1}[\ln(\cosh K_1'/\cosh K_1)+\ln|z_1'-z_1|]+\frac{1}{2mn}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln\mathrm{Det}[\underline{y}_b^{-1}+\underline{G}_b], \tag{4.1}$$

where $f_0(T)$ is the free energy of the perfect lattice given by (2.20), while the determinant of the matrix

$\underline{y}_b^{-1}+\underline{G}_b$, for single-bond defects, can be see from (2.24) to be simply of size 2×2.

In the limit $n, m\to\infty$ we find

$$|\underline{y}_b^{-1}+\underline{G}_b| = \{[0,1]_{RL}^{\infty} - (z_1'-z_1)^{-1}\}^2. \tag{4.2}$$

From the definition (2.25), it is easy to show that the matrix element $[0,1]_{RL}^{\infty}$ has the form

$$[0,1]_{RL}^{\infty} = (1+z_2)tA_{00} + (1-z_2^2)(A_{10}-A_{00}) - 2z_1z_2(A_{01}-A_{00}). \tag{4.3}$$

Using the results of (3.13), (3.20), and (3.21) for the double integrals A_{00}, A_{10}, and A_{01}, we find that the incremental free energy due to a single-bond defect in an infinite lattice is

$$\begin{aligned} f_1^b(T) = {} & \ln(\cosh K_1'/\cosh K_1) + \ln|z_1'-z_1| \\ & + \ln|2(1+z_2)tK(\kappa)/\pi[(t^2+4b)(t^2+4c)]^{1/2} - (2z_1)^{-1}[1-\Lambda_0(\theta,\kappa)] \\ & + z_1(1-z_1^2)^{-1}[1-\Lambda_0(\tilde\theta,\kappa)] - (z_1'-z_1)^{-1}|, \end{aligned} \tag{4.4}$$

where $K(\kappa)$, $\Lambda_0(\theta,\kappa)$, and $\Lambda_0(\tilde\theta,\kappa)$ are the elliptic integral and Heuman's lambda functions introduced after (3.13), (3.20), and (3.22). This result can again be checked by direct calculation for a single bond.[11,12] As $T\to T_c^0$ we find

$$f_1^b(T) \approx \ln|-(1+z_2)\tilde A(t)t\{\ln|t| + \ln 8 + \tfrac12\ln[(b+c)/bc]\} + B(t) + O(t^2\ln|t|)|, \tag{4.5}$$

where

$$B(t) = -\frac{1}{\pi z_1}\tan^{-1}\left(\frac{b}{c}\right)^{1/2} + \frac{2z_1z_2}{\pi c}\tan^{-1}\left(\frac{c}{b}\right)^{1/2} - \frac{1}{z_1'-z_1} \tag{4.6}$$

and $\tilde A(t)$ is given by (3.54). Consequently, the incremental specific heat is

$$C_b^1(T) = -C_0^b/[(T/T_c^0)-1] - C_1^b[\ln|(T/T_c^0)-1|]^2 + O(\ln|t|), \tag{4.7}$$

where

$$C_0^b = r_1(1+z_{2c})\tilde A_c/B_c, \quad C_1^b = (C_0^b)^2, \tag{4.8}$$

in which the subscripts c denote values at $T=T_c^0$, while r_1 is defined by (3.62).

When n and m are finite, we find that the critical point is determined by

$$\begin{aligned} |\underline{y}_b^{-1}(0,0)+\underline{G}_b(0,0)| &= \{[0,1]_{RL}^0 - (z_1'-z_1)^{-1}\}^2 \\ &= \{(1+z_2)tS_{00} + (1-z_2^2)(S_{10}-S_{00}) - 2z_1z_2(S_{01}-S_{00}) - (z_1'-z_1)^{-1}\}^2 = 0. \end{aligned} \tag{4.9}$$

On substituting (3.44), (3.47), and (3.48) for the double sums $S_{pq}(m,n)$, this equation becomes

$$\frac{1+z_{2c}}{tmn} + B_c + \frac{1}{nm}\left[E_3 + \left(\frac{dz_2}{dt}\right)_c\right] + t\tilde A_c(1+z_{2c})[\tfrac12\ln(nm) + P_0(\tau)] + tB_c' + O\left[\frac{\ln(nm)}{n^2m^2}\right] = 0, \tag{4.10}$$

where B_c and B_c' are the first two expansion coefficients of the function $B(t)$ defined in (4.6), namely,

$$B(t) \approx B_c + tB_c' + \cdots, \tag{4.11}$$

while

$$E_3(n/m) = \tfrac12(1+z_{2c})^2z_{2c}^{-1}(n/m)G(\bar n/\bar m) - (m/n)G(\bar m/n), \tag{4.12}$$

where $G(\tau)$ is defined in (3.50). Consequently, the shifted critical temperature has the form

$$T_c^b(x) = T_c^0[1 - Q_1^bx - Q_2^bx^2\ln x^{-1} - Q_3^b(\tau)x^2 - Q_4^bx^3\ln^2x + O(x^3\ln x)], \tag{4.13}$$

with amplitudes

$$Q_1^b = (1+z_{2c})/B_cr_1, \quad Q_2^b = Q_1^b\tilde A_c(1+z_{2c})^2/2B_c^2, \quad Q_4^b = 2(Q_2^b)^2Q_1^b, \tag{4.14}$$

$$Q_3^b\left(\frac{n}{m}\right) = Q_1^b\left\{\frac{B_c'}{B_c^2}(1+z_{2c}) - \frac{1}{B_c}\left[E_3 + \left(\frac{dz_2}{dt}\right)_c\right] + Q_1^b\frac{r_2}{r_1}\right\} + 2Q_2^bP_0(\tau), \tag{4.15}$$

in which $P_0(\tau)$ is defined as before, by letting $t = x/\bar m = y/\bar n \to 0$ in (3.45) with fixed $\bar m$ and $\bar n$. Evidently, the variation of the critical temperature $T_c^b(x)$ for single-bond defects has the same form as for holes. Moreover, its amplitudes Q_1^b and Q_2^c satisfy the corresponding scaling relations[13]

$$C_0 = Q_1^b A_0 \quad \text{and} \quad C_1^b Q_1^b = 2A_0 Q_2^b, \tag{4.16}$$

with $A_0 = r_1^2 \tilde{A}_c$. In a symmetric lattice ($J_1 = J_2 = J$), we find

$$Q_1^b(J_1') = (\sqrt{2} - 1 - z_c')/K_c(2 - \sqrt{2})(\sqrt{2} + 1 + z_c'), \quad Q_2^b(J_1') = 4K_c^2 (Q_1^b)^3/\pi, \tag{4.17}$$

$$Q_3^b(J_1', n/m) = K_c (Q_1^b)^2 \{[\sqrt{2} + (6\sqrt{2} - 4)z_c' - (4 + \sqrt{2})z_c'^2 - 2\sqrt{2}(1 - z_c'^2)(J_1'/J)][1 - 2z_c' - z_c'^2]^{-1} + 4\sqrt{2}[\tfrac{1}{4} - (n/m)G(n/m)] + \tfrac{1}{2}\sqrt{2}(\sqrt{2} - 1)^2\} - (Q_1^b)^2 + 2Q_2^b P_0(\tau). \tag{4.18}$$

This shows that $Q_1^b(J_1') > 0$ for $J_1' < J$ and $Q_1^b(J_1') < 0$ for $J_1' > J$. Hence the shifted critical temperature $T_c(x)$, for a finite concentration x of altered bonds with bond strength $J_1' > J$, is larger than the critical temperature T_c^0 of the pure lattice, but is smaller for $J_1' < J$, in agreement with physical intuition. The numerical values for $J_1' = 0$ are

$$Q_1^b(0) = (\sqrt{2} - 1)/K_c\sqrt{2} \simeq 0.664\,6290,$$

$$Q_2^b(0) = 4K_c^2[Q_1^b(0)]^3/\pi \simeq 0.072\,5952, \tag{4.19}$$

$$Q_4^b(0) \simeq 0.015\,8581,$$

$$Q_3^b(0, 1) \simeq -0.098\,3296, \tag{4.20}$$

$$Q_3^b(0, 2) \simeq -0.374\,4069,$$

$$Q_3^b(0, 3) \simeq -0.616\,1616. \tag{4.21}$$

In the extreme ferromagnetic limit, $J_1' = \infty$, we find likewise

$$Q_1^b(\infty) \simeq -0.664\,6290,$$

$$Q_2^b(\infty) \simeq -0.072\,5952, \tag{4.22}$$

$$Q_4^b(\infty) \simeq -0.015\,8587,$$

$$Q_3^b(\infty, 1) \simeq -0.785\,1338, \tag{4.23}$$

$$Q_3^b(\infty, 2) \simeq -1.111\,530,$$

$$Q_3^b(\infty, 3) \simeq -1.446\,455. \tag{4.24}$$

Finally, in the opposite, antiferromagnetic limit $J_1' = -\infty$ one has

$$Q_1^b(-\infty) = 1/(2 - \sqrt{2})K_c \simeq 3.873\,742,$$

$$Q_2^b(-\infty) \simeq 14.373\,49, \tag{4.25}$$

$$Q_4^b(-\infty) \simeq 106.6654,$$

$$Q_3^b(-\infty, 1) \simeq -33.451\,54, \tag{4.26}$$

$$Q_3^b(-\infty, 2) \simeq -38.703\,26,$$

$$Q_3^b(-\infty, 3) \simeq -39.274\,71. \tag{4.27}$$

B. Bent-bond defects (c): $J_1' = J_2'' = 0$, $J_1'' = J_1$, $J_2' = J_2$

The free energy given by (2.28) for bent, missing double-bond defects, as illustrated in Fig. 2(c), is

$$f(T) = f_0(T) - (nm)^{-1} \ln(\cosh K_1 \cosh K_2) + \frac{1}{2mn} \int_0^{2\pi} \frac{d\theta_1}{2\pi} \int_0^{2\pi} \frac{d\theta_2}{2\pi} \ln[|\underline{y}_c^{-1} + \underline{G}_c|(z_1 z_2)^2], \tag{4.28}$$

where the determinant $|\underline{y}_c^{-1} + \underline{G}_c|$ can be seen from (2.24) to be of size 4×4. It is shown by Ferdinand, in Appendix A, that this determinant can be reduced to a 2×2 determinant, and from (A.21) one finds

$$(z_1 z_2)^2 |\underline{y}_c^{-1} + \underline{G}_c| = [0, 0]_{LL}[0, 0]_{UU} - [0, 0]_{UL}[0, 0]_{LU}. \tag{4.29}$$

Hence, it can be seen from (3.4) and (3.7) that the incremental free energy $f_1^c(T)$ due to a single bent-bond defect in an infinite lattice is

$$\begin{aligned} f_1^c(T) &= -\ln(\cosh K_1 \cosh K_2) + \ln|[0, 0]_{UL}^\infty| \\ &= -\ln(\cosh K_1 \cosh K_2) + \ln\{2tK(\kappa)[1 - z_1 z_2 t(t^2 + 4b + 4c)/8bc]/\pi[(t^2 + 4b)(t^2 + 4c)]^{1/2} \\ &\quad + z_1 z_2 \pi^{-1}(bc)^{-1/2}\kappa^{-1}E + z_1(2b)^{-1}[1 - \Lambda_0(\theta, \kappa)] + z_2(2c)^{-1}[1 - \Lambda_0(\bar{\theta}, \kappa)]\} \\ &= \ln|-\tilde{A}(t)t\{\ln|t| + \ln 8 + \tfrac{1}{2}\ln[(b + c)/bc]\} + \overline{B}(t) + O(t^2 \ln|t|)|, \end{aligned} \tag{4.30}$$

where $K(\kappa)$, $E(\kappa)$, $\Lambda_0(\theta, \kappa)$, and $\Lambda_0(\theta, \bar{\kappa})$ are the elliptic integrals and the Heuman's lambda functions introduced in Sec. III, while $\tilde{A}(t)$ is given in (3.54) and

$$\overline{B}(t) = \frac{z_1}{\pi b} \tan^{-1}\left(\frac{b}{c}\right)^{1/2} + \frac{z_2}{\pi c} \tan^{-1}\left(\frac{c}{b}\right)^{1/2} + \frac{z_1 z_2}{\pi (bc)^{1/2}}. \tag{4.31}$$

Therefore, the incremental specific heat is

$$C_c^1(T) = \frac{-C_0^c}{T/T_c^0 - 1} - C_1^c\left[\ln\left|\frac{T}{T_c^0} - 1\right|\right]^2 + O(\ln|t|), \tag{4.32}$$

with the amplitudes

$$C_0^c = r_1 \tilde{A}_c/\bar{B}_c, \quad C_1^c = (C_0^c)^2: \tag{4.33}$$

in which the subscript c again denote values evaluated at $T = T_c$.

When n, m are finite, using (4.29), (3.37), and (3.40) we find that the critical temperature is determined by

$$[0,0]_{UL}^0 = tS_{00} - z_1(S_{10} - S_{00}) - z_2(S_{01} - S_{00}) - z_1 z_2(S_{11} - S_{00}) = 0. \tag{4.34}$$

On substituting (3.44) and (3.47)–(3.49) for the double sums $S_{pq}(m,n)$, this equation reduces to

$$(tmn)^{-1} + \bar{B}_c + (nm)^{-1}E_4 + t\left[\tfrac{1}{2}\tilde{A}_c \ln(nm) + \tilde{A}_c P_0(\tau) + \bar{B}_c'\right] + O[n^{-2}m^{-2}\ln(nm)] = 0, \tag{4.35}$$

where, simply,

$$\bar{B}_c = \bar{B}(0), \quad \bar{B}_c' = \left(\frac{d\bar{B}}{dt}\right)_{t=0}, \tag{4.36}$$

while

$$E_4\left(\frac{n}{m}\right) = -\frac{1+z_{2c}}{2z_{2c}}\left(\frac{n}{m}\right)G\left(\frac{\bar{n}}{\bar{m}}\right) - \frac{1+z_{1c}}{2z_{1c}}\left(\frac{m}{n}\right)G\left(\frac{\bar{m}}{\bar{n}}\right), \tag{4.37}$$

in which $G(\tau)$ is defined in (3.50). Hence we find the result

$$T_c^c(x) = T_c\left[1 - Q_1^c x - Q_2^c x^2 \ln x^{-1} - Q_3^c(n/m)x^2 - Q_4^c x^3 \ln^2 x + O(x^3 \ln x)\right], \tag{4.38}$$

with

$$Q_1^c = \frac{1}{r_1 \bar{B}_c}, \quad Q_2^c = \frac{\tilde{A}_c}{2r_1 \bar{B}_c^3}, \quad Q^c = \frac{2(Q_2^c)^2}{Q_1^c}, \tag{4.39}$$

$$Q_3^c\left(\frac{n}{m}\right) = Q_1^c\left(\frac{-E_4}{\bar{B}_c} + \frac{\bar{B}_c'}{\bar{B}_c^2}\right) + 2Q_2^c P_0(\tau) + \frac{(Q_1^c)^2 r_2}{r_1}, \tag{4.40}$$

which again satisfy the predicted scaling relations

$$Q_1^c = C_0^c/A_0, \quad Q_2^c = \tfrac{1}{2}A_0(Q_1^c)^3 = \tfrac{1}{2}C_1^c Q_1^c/A_0. \tag{4.41}$$

The numerical values for a symmetric lattice ($J_1 = J_2$) are

$$Q_1^c = 1/K_c 2\sqrt{2}\left[\tfrac{1}{2} + (\sqrt{2} - 1)/\pi\right] \simeq 1.267\,973, \tag{4.42}$$

$$Q_2^c \simeq 0.506\,1820, \quad Q_4^c \simeq 0.404\,1414, \tag{4.43}$$

$$Q_3^c(1) \simeq -0.679\,9627, \quad Q_3^c(2) \simeq -0.504\,5234, \quad Q_3^c(3) \simeq -0.179\,7111. \tag{4.44}$$

C. Straight-bond defects (d): $J_1'' = J_1' = 0$, $J_2' = J_2'' = J_2$

Finally, we consider the case of a straight double-bond defect as illustrated in Fig. 2(d). The free energy of (2.28) can be written as a double integral over the logarithm of a 4×4 determinant, namely,

$$f(T) = f_0(T) + \frac{1}{nm}\ln\sinh^2 K_1 + \frac{1}{2mn}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln|\underline{y}_d^{-1} + \underline{G}_d|. \tag{4.45}$$

In the limit $n, m \to \infty$, the matrix $\underline{y}_d^{-1} + \underline{G}_d$ becomes antisymmetric and we find that the incremental free energy due to a single straight-bond defect is

$$f_1^d(T) = 2\ln\sinh K_1 + \ln|(z_1^{-1} + [0,1]_{RL}^\infty)^2 - [0,0]_{RL}^\infty[0,2]_{RL}^\infty|, \tag{4.46}$$

where $[0,0]_{RL}^\infty$ is given by (3.5) and $[0,1]_{RL}^\infty$ by (4.3), while we have

$$[0,2]_{RL}^\infty = (1+z_2)tA_{00} + (1 - z_2^2)(A_{20} - A_{00}) - z_1(1 + z_2^2)(A_{10} - A_{00}) - 2z_1 z_2(A_{11} - A_{00}). \tag{4.47}$$

It is easy to verify the relation

$$aA_{10} - b(A_{20} + A_{00}) - 2cA_{11} = 0. \tag{4.48}$$

This shows that $[0,2]_{RL}^\infty$ can also be written in terms of the double integrals already calculated in Sec. III. In fact, we find

$$[0,2]_{RL}^\infty = 2tK[(1+z_2) + tz_1^{-1} - tz_2(t^2 + 4b + 4c)(4z_1 bc)^{-1}]/\pi[(t^2 + 4b)(t^2 + 4c)]^{1/2} - (1 + z_2^2)(2z_1 b)^{-1}[1 - \Lambda_0(\theta,\kappa)] + 2z_2 z_1^{-1}\kappa^{-1}E/\pi(bc)^{1/2}. \tag{4.49}$$

As $T\to T_c^0$ $(t\to 0)$, the incremental free energy thus varies according to

$$f_1^d(T)=\ln|\bar{D}_0(t)-\bar{D}_1(t)t\,\{\ln|t|+\ln 8+\tfrac{1}{2}\ln[(b+c)/bc]\}+O(t^2\ln|t|)|, \tag{4.50}$$

where the amplitudes $\bar{D}_0(t)$ and $\bar{D}_1(t)$ are again analytic functions of t and are listed in Table II. The incremental specific heat due to a isolated straight-double-bond defect is

$$C_1^d(T)=\frac{-C_0^d}{T/T_c^0-1}-C_1^d\left[\ln\left|\frac{T}{T_c^0}-1\right|\right]^2+O(\ln|t|) \tag{4.51}$$

in which the amplitudes are

$$C_0^d=r_1\bar{D}_{1c}/\bar{D}_{0c},\quad C_1^d=(C_0^d)^2. \tag{4.52}$$

When n and m are finite, we can, by using a relation similar to (4.48), namely,

$$aS_{10}-b(S_{00}+S_{20})-2cS_{11}=0, \tag{4.53}$$

show that the critical equation

$$|\underline{y}_d^{-1}(0,0)+\underline{G}_d(0,0)|=0 \tag{4.54}$$

reduces to

$$\bar{D}_0(t)+\bar{D}_1(t)\tilde{A}(t)^{-1}tS_{00}+(tn^2m^2)^{-1}E_5+(nm)^{-1}E_6+O(n^{-2}m^{-2}\ln n)=0, \tag{4.55}$$

where $\tilde{A}(t)$ is defined in (3.54), $\bar{D}_0(t)$ and $\bar{D}_1(t)$ listed in Table II, $E_5\equiv 0$, and $E_6(n/m)$ given in Table III. Consequently, we obtain for $T_c^d(x)$ a result of the same form as before but with amplitudes

$$Q_1^d=\frac{\bar{D}_{1c}}{\bar{D}_{0c}\tilde{A}_c r_1},\quad Q_2^d=\frac{\frac{1}{2}\bar{D}_{1c}^3}{\bar{D}_{0c}^3\tilde{A}_c^2 r_1},\quad Q_4^d=\frac{2(Q_2^d)^2}{Q_1^d}, \tag{4.56}$$

$$Q_3^d\left(\frac{n}{m}\right)=Q_1^d\{(\bar{D}_{1c}/\tilde{A}_c)\bar{D}'_{0c}/\bar{D}_{0c}^2-\bar{D}_{0c}^{-1}[E_6(n/m)+(\bar{D}_1/\tilde{A})'_c]+Q_1^d r_2/r_1\}+2Q_2^d P_0(\tau), \tag{4.57}$$

in which the prime denotes the derivative with respect to t and the subscript c denotes values at $T=T_c^0$; $P_0(\tau)$ is defined as before by letting $t=x/\bar{m}=y/\bar{n}\to 0$ in (3.45) with fixed $\bar{m}$ and $\bar{n}$, and r_1, r_2 are defined in (3.62). The appropriate scaling relations are again satisfied.

In a symmetric lattice $(J_1=J_2=J)$, we find the numerical values

$$Q_1^d=\frac{1-2\sqrt{2}-1)/\pi}{[\sqrt{2}-4(\sqrt{2}-1)/\pi^2]K_c}\simeq 1.141\,706, \tag{4.58}$$

$$Q_2^d\simeq 0.367\,9879,\quad Q_4^d\simeq 0.237\,2154, \tag{4.59}$$

$$Q_3^d(1)\simeq -1.169\,508,$$
$$Q_3^d(2)\simeq -1.629\,508, \tag{4.60}$$
$$Q_3^d(3)\simeq -1.955\,392.$$

V. DISCUSSION

We may summarize our analysis of the shift in critical temperature produced by an array of point defects on an $m\times n$ grid by the rather simple expression

$$T_c(x,\tau)=T_c^0[1-(C_0/A_0)x-\tfrac{1}{2}(C_0^3/A_0^2)x^2\ln x^{-1}-Q_3(\tau)x^2-\tfrac{1}{2}(C_0^5/A_0^3)x^3\ln^2 x+O(x^3\ln x)], \tag{5.1}$$

where $x=1/nm$ is the density of defects (on a per site basis) and $\tau=n/m$. The amplitudes A_0 and C_0 are those of the leading critical singularities in the bulk specific heat and in the incremental specific heat due to a single isolated defect [see (1.2) and (1.3)]. To derive this expression we have observed that $C_1=C_0^2$, which follows from (3.30), (4.8), (4.33), and (4.52).[22] The form (5.1) is consistent with a general scaling theory[13] for the effect of point defects; thus although it has been checked explicitly only for the defects illustrated in Fig. 2, we expect it to be true for all bounded defects in the limit of low density. A further check on the scaling theory is provided in the following paper[14] where the change in the *amplitude* of the shifted logarithmic specific-heat singularity is calculated.

It is instructive to examine the results for the various defects numerically; this indeed reveals that the asymptotic form (5.1) is surprisingly accurate even for concentrations x so large that the mean defect spacing is only two lattice spacings! To compare the different defects in the case where the modified interactions are all zero, corresponding to missing bonds, it is useful to to introduce $\tilde{x}$, the fraction of missing bonds (per bond) via the definition

$$\begin{aligned}\tilde{x}&=2x \text{ for vacancies } (a),\\ &=\tfrac{1}{2}x \text{ for missing single bonds } (b),\\ &=x \text{ for missing double bonds } (c) \text{ and } (d).\end{aligned} \tag{5.2}$$

The corresponding reductions in T_c according to our asymptotic formula (5.1) are plotted versus

$\tilde{x}$ in Fig. 3, for a symmetric lattice ($J_1 = J_2$) with a square grid of defects ($m=n$, $\tau=1$). In this normalization the tighter groupings of missing bonds yield higher critical temperatures, as is to be expected. The close similarity of the single-bond and bent-double-bond defects [(b) and(c)] is, however, rather surprising. We may note that for missing single bonds we find $[T_c(x)/T_c^0]-1 \approx 2Q_1^b \tilde{x} \simeq 1.329\,258\tilde{x}$, in leading order; this agrees with Harris's result for a random system of missing bonds.[1] Since the coefficient of x is *independent* of the distribution ratio τ it is quite reasonable that the random- and ordered-system shifts in T_c should agree in first order.

The dependence of $T_c(x, \tau)$ on the distribution ratio for vacancies is shown in Fig. 4, which displays the deviation from the leading linear form $T_c^0(1-Q_1 x)$. The critical-temperature depression is smallest for a square defect array. It is remarkable, however, that even for a mean spacing as small as $3\frac{1}{2}$ lattice constants, the critical point varies over only 0.8% as the distribution ratio increases up to 3:1.

By symmetry we have $T_c(x, \tau) = T_c(x, \tau^{-1})$ for vacancies and bent-bond defects. However, this is not the case for the oriented, anisotropic defects (b) and (d), as can be seen from Fig. 5. For single-bond defects it is clear that the lattice decomposes into disconnected vertical strips of finite width m when $n=1$. For such configurations one must have $T_c \equiv 0$; the same argument applies to straight-double-bond defects when $n=1$. These observations provide an understanding of why the critical temperatures at fixed x fall rapidly when τ ($=1/m$) decreases, as evident in Fig. 5. We may note in passing that bent double bonds (c) with m or n equal to unity also yield $T_c \equiv 0$. For vacancies, however, the lowest values $m = n = 2$, $x = \frac{1}{4}$ leave the lattice two dimensional and hence with a finite T_c. [By contrast a *random* distribution of vacancies at a density exceeding the percolation density p_c ($\simeq 0.55$) disconnects the lattice into finite pieces with probability one and hence yields $T_c(x) \equiv 0$ for $x > p_c$.]

Finally, to demonstrate the accuracy of the asymptotic expression for $T_c(x)$ at finite x we examine the values of T_c for various small finite values of m and n (which leave the lattice two-dimensionally connected). Consider first single-

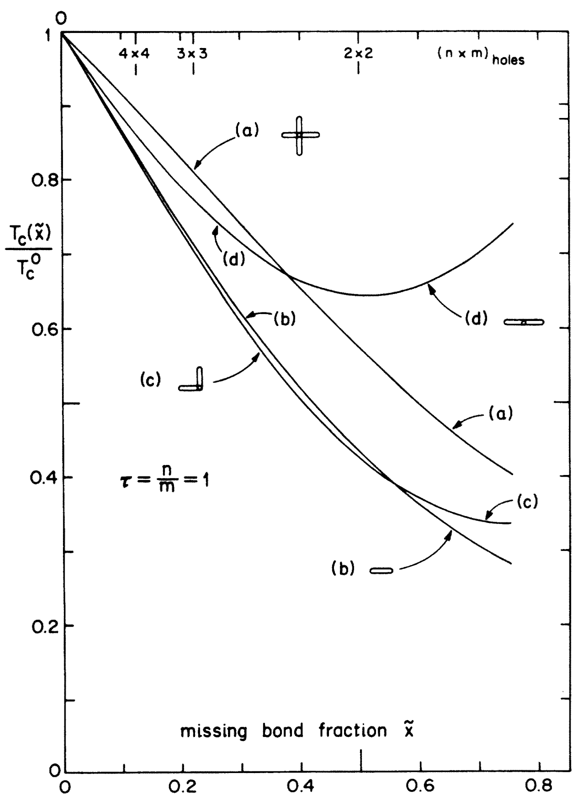

FIG. 3. Shift in critical temperature of a symmetric lattice ($J_1 = J_2$) produced by vacancies and missing-bond defects distributed on a regular $m \times n$ array vs the missing-bond fraction $\tilde{x} \propto 1/mn$, according to the asymptotic formula (5.1).

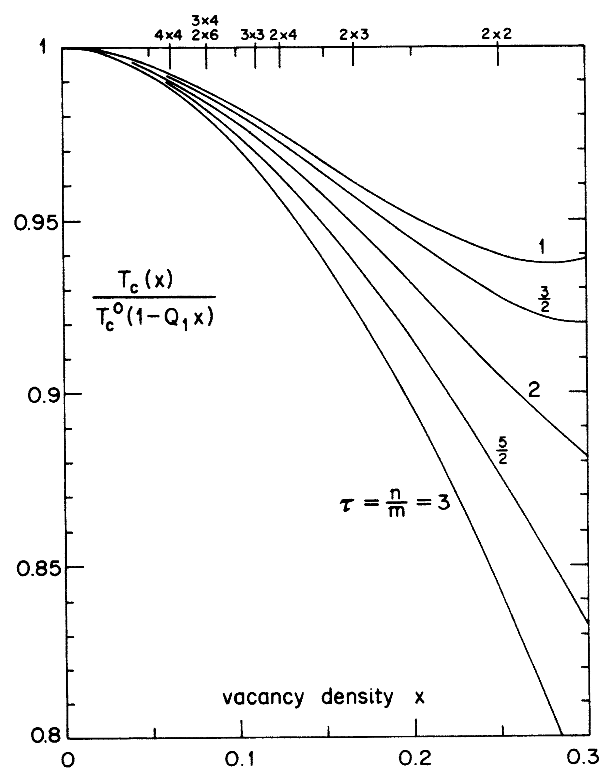

FIG. 4. Shift in critical temperature vs concentration x produced by vacancies on $m \times n$ array for different values of $\tau = n/m$. Note that the τ-independent linear shift has been divided out.

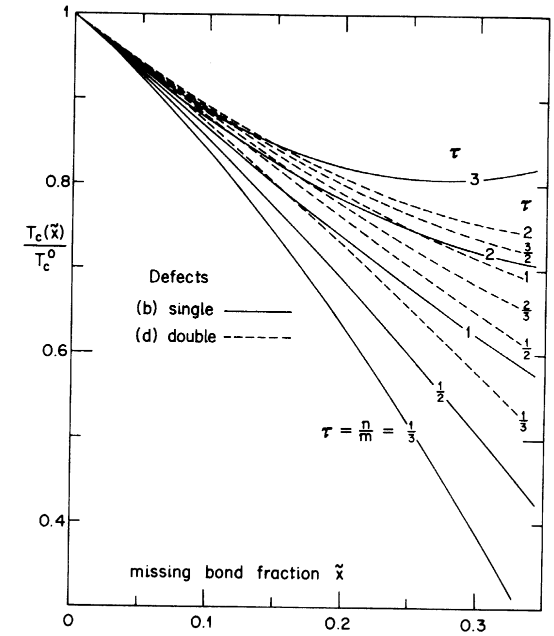

FIG. 5. Variation of critical temperature with distribution ratio $\tau = n/m$ for missing single-bond defects (b) (solid lines) and straight-double-bond defects (d) (dashed curves).

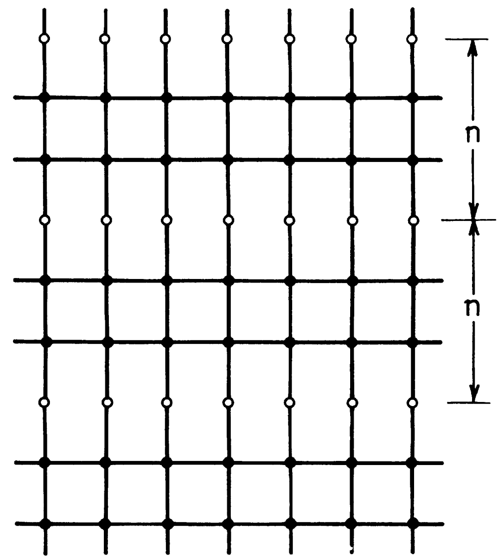

FIG. 6. A lattice with single-bond defects (b) on a grid with $m = 1$ or, equivalently, double-bond defects (d) on a grid with $m = 2$.

bond defects (b) and straight-double-bond defects (d), with $m = 1$ and 2, respectively, but n arbitrary. As can be seen from Fig. 6, these yield the *same* configuration of missing bonds so that $T_c^b(m=1, n) \equiv T_c^d(m=2, n)$. Furthermore, by using the decoration technique[12] to remove the sites adjacent to the missing bonds, this lattice structure can be reduced to a *layered lattice*.[23] The critical temperatures of arbitrary layered Ising models can be found exactly.[4,23] In this way the critical equations are seen to be

$$(1 - z_1)/(1 + z_1) = z_2^{n/(n-1)}. \tag{5.3}$$

The exact critical temperatures following by solution of these equations for $n = 2$–6 are displayed in Table IV. Also listed in the table are the percentage deviations from the exact results obtained by using the asymptotic formula (5.1) (with appropriate m and n), both retaining the term of order $x^3 \ln x^2$, and truncating the expansion at order x^2. In the worst case the deviation

TABLE IV. Exact values of $T_c(x, \tau)/T_c^0$ in a symmetric lattice with $\tau = n/m$ for single-missing-bond (b) and straight, double-missing-bond (d) defects, compared with the asymtotic expansion (1.4) truncated at $O(x^3 \ln^2 x)$ and $O(x^2)$.

		Exact	(b) $m=1$, $x=2\tilde{x}$ Percentage deviation		(d) $m=2$, $x=\tilde{x}$ Percentage deviation	
n	$\tilde{x}$	$T_c(x, \tau)/T_c^0$	$O(x^3 \ln^2 x)$	$O(x^2)$	$O(x^3 \ln^2 x)$	$O(x^2)$
2	0.25	0.723 1749	3.399	3.531	3.527	4.512
3	$0.1\dot{6}$	0.822 8277	1.765	1.851	0.592	1.021
4	0.125	0.869 4034	1.266	1.321	−0.071	0.160
5	0.1	0.896 5256	0.989	1.026	−0.271	−0.130
6	$0.08\dot{3}$	0.914 3005	0.817	0.842	−0.335	−0.242

TABLE V. Critical-point equations for vacancies at spacings $m \times n$ [from Ferdinand (unpublished)].

2×2	$(1-z_2^2)=z_1^2(1+z_2^2)$
2×3	$(1-z_2^2)^2=z_1^3(1+6z_2^2+z_2^4)$
2×4	$(1-z_2^2)^4=z_1^4(1+15z_2^2+15z_2^4+z_2^6)$
2×5	$(1-z_2^2)^5=z_1^5(1+28z_2^2+70z_2^4+28z_2^6+z_2^8)$

is only a few percent and, as $\bar{x}$ decreases to 0.1, this error drops rapidly below 1%. (The expression for double-bond defects gives better agreement, presumably because x is $1/2n$ in that case rather than $1/n$.)

The decoration technique can also be used easily to find the exact T_c for vacancies on a 2×2 grid. For larger values of (m, n) the critical temperature can, in principle, be found from the determinantal equation

$$\mathrm{Det}\underline{\mathrm{U}}(0, 0; T)=0, \tag{5.4}$$

where $\underline{\mathrm{U}}(\theta_1, \theta_2; T)$ is the $4mn\times 4mn$ matrix specified by (2.10). However, owing to the rapidly increasing size of these determinants their algebraic reduction is somewhat tricky. Nevertheless, with perseverence one may obtain the explicit critical-point equations displayed in Table V for the $2\times n$ sequence with $n=2$–5. The exact critical temperatures for vacancies following from these equations are listed in Table VI. Also shown in this table are the percentage deviations from the exact values resulting from evaluation of (5.1) correct to orders $x^3\ln^2 x$ and x^2, respectively. The full expression is in error by less than 1% even for $m=n=2$, which is the most concentrated case realizable! The deviation drops below $\frac{1}{3}\%$ as x decreases to 0.1. Furthermore, the true values are bracketed by the expressions truncated at $O(x^2)$ and $O(x^3\ln^2 x)$. The asymptotic expansion is thus very satisfactory for $x< 0.1$.

TABLE VI. Exact values of $T_c(x,\tau)/T_c^0$ in a symmetric lattice with $\tau=n/m$ for vacancies (a), compared with the asymptotic expansion (1.4) truncated at $O(x^3\ln^2 x)$ and $O(x^2)$.

$m\times n$	x	Exact $T_c(x,\tau)/T_c^0$	Percentage deviation $O(x^3\ln^2 x)$	$O(x^2)$
2×2	0.25	0.576 5997	−0.816	5.159
2×3	$0.16\dot{6}$	0.711 7460	−0.615	1.781
2×4	0.125	0.782 0642	−0.436	0.803
2×5	0.1	0.824 8923	−0.326	0.411

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APPENDIX A: REDUCTION OF THE GREEN'S-FUNCTION DETERMINANTS

In evaluating the thermodynamic properties of a diagonal interface in a lattice and a diagonal lattice edge,[16] it is found that the matrix elements $[l,k]_{\lambda\mu}$ satisfy many useful interrelationships. These relationships will be demonstrated here. Using them, we can also show that the determinant $|\underline{\mathrm{y}}^{-1}+\underline{\mathrm{G}}|$ for holes, or for bent-bond defects (Fig. 2), can be reduced in size by a factor of 2.

If $g=1+z_1e^{i\phi_1}$ and $h=1+z_2e^{i\phi_2}$ [see (2.25)] it is straightforward to verify the two identities

$$h+h^*+z_1^{-1}[(h+h^*-ghh^*)-(2-gh^*)]e^{-i\phi_1} - (z_2/z_1)(2-gh)e^{i\phi_1-i\phi_2}=0\,, \tag{A1}$$

$$(-2+g^*h)e^{i\phi_1}+z_1^{-1}[(2-gh)+(g-g^*)] -(z_2/z_1)(g+g^*-gg^*h)e^{-i\phi_2}=z_1^{-1}\Delta(\phi_1,\phi_2)\,, \tag{A2}$$

where Δ is defined in (2.19). It can be seen from the definition (2.25) of the matrix element $[l,k]_{\lambda\mu}$ that (A1) implies

$$[s,s']_{RR}+z_1^{-1}([s,s'+1]_{RL}-[s,s'+1]_{RU}) - (z_2/z_1)[s+1,s'+1]_{RD}=0\,, \tag{A3}$$

and

$$[s+1,s'+1]_{UL}-z_2^{-1}([s,s'+1]_{DL}+[s,s'+1]_{RL}) +(z_1/z_2)[s,s']_{LL}=0\,. \tag{A4}$$

Likewise (A2) yields

$$[s,s'-1]_{UR}+z_1^{-1}([s,s']_{UL}-[s,s']_{UU}) +(z_2/z_1)[s,s'-1]_{UD}=z_1^{-1}\delta_{s,0}\delta_{s',0} \tag{A5}$$

and

$$[s+1,s']_{UD}-z_2^{-1}([s,s']_{DD}+[s,s']_{RD}) +(z_1/z_2)[s,s'-1]_{LD}=z_1^{-1}\delta_{s,0}\delta_{s',0}\,. \tag{A6}$$

On taking the complex conjugate of both sides of (A1) and (A2), we obtain two further equations, each of which gives rise to two equations that relate the elements $[l,k]_{\lambda\mu}$. Next, we can see from the definition of g and h that we may interchange z_1 and z_2, and ϕ_1 and ϕ_2, in (A1) and (A2). The resulting equations and their complex conjugates give rise to eight further equations for $[l,k]_{\lambda\mu}$. These 16 equations can be summarized by the four matrix equations

$$\underline{Q}(s,s')\begin{bmatrix}1\\ z_1^{-1}\\ -z_1^{-1}\\ -z_2/z_1\end{bmatrix}=\begin{bmatrix}0\\ z_1^{-1}\\ z_1^{-1}\\ 0\end{bmatrix}\delta_{s,0}\delta_{s',0},\qquad \underline{Q}^T(s,s')\begin{bmatrix}1\\ z_1^{-1}\\ -z_1^{-1}\\ -z_1/z_2\end{bmatrix}=\begin{bmatrix}0\\ -z_1^{-1}\\ -z_1^{-1}\\ 0\end{bmatrix}\delta_{s,0}\delta_{s',0}. \tag{A7}$$

and

$$\underline{\bar{Q}}(s,s')\begin{bmatrix}1\\ -z_2^{-1}\\ -z_2^{-1}\\ z_1/z_2\end{bmatrix}=\begin{bmatrix}0\\ z_2^{-1}\\ -z_2^{-1}\\ 0\end{bmatrix}\delta_{s,0}\delta_{s',0},\qquad \underline{\bar{Q}}^T(s,s')\begin{bmatrix}1\\ -z_2^{-1}\\ -z_2^{-1}\\ z_1/z_2\end{bmatrix}=\begin{bmatrix}0\\ -z_2^{-1}\\ z_2^{-1}\\ 0\end{bmatrix}\delta_{s,0}\delta_{s',0}, \tag{A8}$$

where the Green's-function matrices are

$$\underline{Q}(s,s')=\begin{bmatrix}[s,s']_{RR} & [s,s'+1]_{RL} & [s,s'+1]_{RU} & [s+1,s'+1]_{RD}\\ [s,s'-1]_{LR} & [s,s']_{LL} & [s,s']_{LU} & [s+1,s']_{LD}\\ [s,s'-1]_{UR} & [s,s']_{UL} & [s,s']_{UU} & [s+1,s']_{UD}\\ [s-1,s'-1]_{DR} & [s-1,s']_{DL} & [s-1,s']_{DU} & [s,s']_{DD}\end{bmatrix}, \tag{A9}$$

$$\underline{\bar{Q}}(s,s')=\begin{bmatrix}[s,s']_{UU} & [s+1,s']_{UD} & [s+1,s']_{UR} & [s+1,s'+1]_{UL}\\ [s-1,s']_{DU} & [s,s']_{DD} & [s,s']_{DR} & [s,s'+1]_{DL}\\ [s-1,s']_{RU} & [s,s']_{RD} & [s,s']_{RR} & [s,s'+1]_{RL}\\ [s-1,s'-1]_{LU} & [s,s'-1]_{LD} & [s,s'-1]_{LR} & [s,s']_{LL}\end{bmatrix}, \tag{A10}$$

while the superscript T denotes the matrix transpose.

We can now use (A7) and (A8) to reduce the size of the determinant $|\underline{y}^{-1}+\underline{G}|$ for holes. We find from (2.23) and (2.24) that the 8×8 matrix $\underline{y}^{-1}$ can be put in the form

$$\underline{y}^{-1}=\underline{V}^*\begin{bmatrix}\underline{y}_1^{-1} & 0\\ 0 & \underline{y}_2^{-1}\end{bmatrix}\underline{V}, \tag{A11}$$

where

$$\underline{V}=\begin{bmatrix}\underline{U}(\theta_2) & 0\\ 0 & \underline{U}(\theta_1)\end{bmatrix}\ \text{with}\ \underline{U}(\theta)=\begin{bmatrix}1 & & & \\ & 1 & & \\ & & 1 & \\ & & & e^{i\theta}\end{bmatrix}, \tag{A12}$$

and

$$\underline{y}_1^{-1}=\begin{bmatrix}0 & z_1^{-1} & 0 & 0\\ -z_1^{-1} & 0 & 0 & 0\\ 0 & 0 & 0 & z_2^{-1}\\ 0 & 0 & -z_2^{-1} & 0\end{bmatrix},\qquad \underline{y}_2^{-1}=\begin{bmatrix}0 & z_2^{-1} & 0 & 0\\ -z_2^{-1} & 0 & 0 & 0\\ 0 & 0 & 0 & z_1^{-1}\\ 0 & 0 & -z_1^{-1} & 0\end{bmatrix}. \tag{A13}$$

From the definition (2.25) of the matrix elements $[l,k]_{\lambda\mu}$ we obtain the following relations:

$$[l,k\pm m]_{\lambda\mu}=e^{\mp i\theta_1}[l,k]_{\lambda\mu},\quad [l\pm n,m]_{\lambda\mu}=e^{\mp i\theta_2}[l,k]_{\lambda\mu}. \tag{A14}$$

These equations together with (2.24) show that the 8×8 basic Green's-function matrix $\underline{G}$ has the form

$$\underline{G} = \underline{V}^* \begin{bmatrix} \underline{Q}(0,0) & \underline{Y} \\ \underline{X} & \overline{\underline{Q}}(0,0) \end{bmatrix} \underline{V} , \tag{A15}$$

where $\underline{Q}$ and $\overline{\underline{Q}}$ are given by (A9) and (A10), while

$$\underline{X} = \begin{bmatrix} [1,-1]_{UR} & [1,0]_{UL} & [1,0]_{UU} & [2,0]_{UD} \\ [0,-1]_{DR} & [0,0]_{DL} & [0,0]_{DU} & [1,0]_{DD} \\ [0,-1]_{RR} & [0,0]_{RL} & [0,0]_{RU} & [1,0]_{RD} \\ [0,-2]_{LR} & [0,-1]_{LL} & [0,-1]_{LU} & [1,-1]_{LD} \end{bmatrix} , \tag{A16}$$

$$\underline{Y} = \begin{bmatrix} [-1,1]_{RU} & [0,1]_{RD} & [0,1]_{RR} & [0,2]_{RL} \\ [-1,0]_{LU} & [0,0]_{LD} & [0,0]_{LR} & [0,1]_{LL} \\ [-1,0]_{UU} & [0,0]_{UD} & [0,0]_{UR} & [0,1]_{UL} \\ [-2,0]_{DU} & [-1,0]_{DD} & [-1,0]_{DR} & [-1,1]_{DL} \end{bmatrix} . \tag{A17}$$

Note that the rows of $\underline{X}$ and $\underline{Y}$ are rows of either $\underline{Q}(1,0)$ or $\underline{Q}(0,-1)$ and either $\underline{Q}(0,1)$ or $\overline{\underline{Q}}(-1,0)$, respectively, while the columns of $\underline{X}$ and $\underline{Y}$ are columns of either $\overline{\underline{Q}}(0,-1)$ or $\overline{\underline{Q}}(1,0)$ and either $\underline{Q}(-1,0)$ or $\underline{Q}(0,1)$, respectively. Since the rows of columns of $\underline{Q}$ and $\overline{\underline{Q}}$ satisfy the matrix equations (A1) and (A8), we can apply row operations and column operations to the determinant $|\underline{y}^{-1}+\underline{G}|$ to reduce its size. To be specific, we first multiply the matrix $\underline{V}(\underline{y}^{-1}+\underline{G})\underline{V}^*$ from the right by a constant matrix block diagonal matrix $\underline{K}=\mathrm{diag}\{\underline{K}_1, \underline{K}_2\}$ where

$$\underline{K}_1 = \begin{bmatrix} 1 & & & \\ z_1^{-1} & 1 & & \\ -z_1^{-1} & 0 & 1 & \\ -z_2/z_1 & 0 & 0 & 1 \end{bmatrix} ,$$

$$\underline{K}_2 = \begin{bmatrix} 1 & & & \\ -z_2^{-1} & 1 & & \\ -z_2^{-1} & 0 & 1 & \\ z_1/z_2 & 0 & 0 & 1 \end{bmatrix} , \tag{A18}$$

and then multiply it from the left by the transpose matrix $\underline{K}^T$. This leads to

$$|\underline{y}^{-1}+\underline{G}| = |\underline{K}^T\underline{V}(\underline{y}^{-1}+\underline{G})\underline{V}^*\underline{K}|$$
$$= (z_1z_2)^{-4}|[0,0]_{\lambda\mu}| , \quad \lambda, \mu = R, L, U, D , \tag{A19}$$

which completes the reduction.

Consider now the case of a bent-double-bond defect [Fig. 2(c)] specified by $J_1' = J_2'' = 0$, $J_1'' = J_1$, $J_2' = J_2$. It is not hard to see that the matrix $(\underline{y}_c^{-1}+\underline{G}_c)$ for the perpendicular missing bonds is a submatrix of the matrix $\underline{y}^{-1}+\underline{G}$ for holes. In fact, from (2.24) we find

$$\underline{y}_c^{-1}+\underline{G}_c = \underline{U}^*(\theta)[\underline{y}_1^{-1}+\underline{Q}(0,0)]\,\underline{U}(\theta) . \tag{A20}$$

Consequently, on using (A7) we have

$$|y_c^{-1}+G| = |\underline{K}_1^T[\underline{y}^{-1}+\underline{Q}(0,0)]\,\underline{K}_1|$$
$$= (z_1z_2)^{-2} \begin{vmatrix} [0,0]_{LL} & [0,0]_{LU} \\ [0,0]_{UL} & [0,0]_{UU} \end{vmatrix} , \tag{A21}$$

which is only a 2×2 determinant.

APPENDIX B: DOUBLE SUMS $S_{pq}\ (m,n)$

In analyzing the double sums S_{pq}, we find that it is possible to carry out one of the summations exactly. Hence we first calculate a sum of the form

$$I = n^{-1}\sum_{l=1}^{n}\left[x - y\cos\left(\frac{2\pi l}{n}\right) - z\sin\left(\frac{2\pi l}{n}\right)\right]^{-1} , \tag{B1}$$

with $x^2 \geqslant y^2 + z^2$. The summand $r(\theta)$ has the Fourier series

$$r(\theta) = r_0 + \sum_{l=1}^{\infty}(r_l + r_{-l})e^{il\theta} , \tag{B2}$$

whose coefficients can be easily found as

$$r_{\pm|l|} = (x^2 - y^2 - z^2)^{-1/2}\{(y \pm iz)/[x + (x^2 - y^2 - z^2)^{1/2}]\}^{|l|}. \tag{B3}$$

Consequently, the sum becomes[24]

$$I = r_0 + \sum_{l=1}^{\infty} (r_{nl} + r_{-nl}) \tag{B4}$$

$$= (x^2 - y^2 - z^2)^{-1/2}\left\{1 + \frac{1}{[x + (x^2 - y^2 - z^2)^{1/2}]^n/(y - iz)^n - 1} + \frac{1}{[x + (x^2 - y^2 - z^2)^{1/2}]^n/(y + iz)^n - 1}\right\}. \tag{B5}$$

On using this result, we find

$$S_{00} = m^{-1}\sum_{l=1}^{m} n^{-1}\sum_{k=1}^{n}\left[a - 2b\cos\left(\frac{2\pi l}{m}\right) - 2c\cos\left(\frac{2\pi k}{n}\right)\right]^{-1},$$

$$= m^{-1}\sum_{l=1}^{m} X\left(\frac{2\pi l}{m}\right)^{-1}\left[1 + 2\Big/ Y\left(\frac{2\pi l}{m}\right)\right], \tag{B6}$$

where

$$X(\theta) = ([a - 2b\cos\theta]^2 - 4c^2)^{1/2}, \tag{B7}$$

$$Y(\theta) = \left(\frac{[a - 2b\cos\theta]}{2c} + \frac{X(\theta)}{2c}\right)^n - 1, \tag{B8}$$

and

$$S_{10} = m^{-1}\sum_{l=1}^{m}\cos\left(\frac{2\pi l}{m}\right) X\left(\frac{2\pi l}{m}\right)^{-1}\left[1 + 2\Big/ Y\left(\frac{2\pi l}{m}\right)\right]. \tag{B9}$$

Since we can write

$$\frac{\cos(2\pi k/n)}{a - 2b\cos(2nl/m) - 2c\cos(2\pi k/n)}$$

$$= -(2c)^{-1} + \frac{a - 2b\cos(2\pi l/m)}{2c[a - 2b\cos(2\pi l/m) - 2c\cos(2\pi k/n)]}, \tag{B10}$$

we have

$$S_{01} = -(2c)^{-1} + (a/2c)S_{00} - (b/c)S_{10}, \tag{B11}$$

and also

$$S_{11} = \frac{a}{2c}S_{10} - \frac{b}{c}\sum_{l=1}^{m}\cos^2\left(\frac{2\pi l}{m}\right) X\left(\frac{2\pi l}{m}\right)^{-1}\left[1 + 2\Big/ Y\left(\frac{2\pi l}{m}\right)\right]. \tag{B12}$$

For $j = 1, 2, 3$ let us put

$$I_j = \frac{1}{m}\sum_{l=1}^{m}\cos^{j-1}\left(\frac{2\pi l}{m}\right)\Big/ X\left(\frac{2\pi l}{m}\right), \tag{B13}$$

$$J_j = \frac{1}{m}\sum_{l=1}^{m}\cos^{j-1}\left(\frac{2\pi l}{m}\right)\Big/ X\left(\frac{2\pi l}{m}\right) Y\left(\frac{2\pi l}{m}\right). \tag{B14}$$

We shall calculate these sums individually in the limit $n, m \to \infty$ (fixed τ) as $t \to 0$.

Sums I_j

We can write

$$X(\theta) = \{t^2 + 4b\sin^2(\tfrac{1}{2}\theta)\}^{1/2}\{t^2 + 4c + 4b\sin^2(\tfrac{1}{2}\theta)\}^{1/2}, \tag{B15}$$

in which t is given by (3.18); then we can make the decomposition

$$I_1 \equiv I_1^a + I_1^b + R_1 + R_2, \tag{B16}$$

where the contributions in order of importance are

$$I_1^a = (2mc^{1/2})^{-1}\sum_{l=1}^{m}\left[t^2 + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}, \tag{B17}$$

$$I_1^b=(4mb^{1/2})^{-1}\sum_{l=1}^{m}\left[\sin\left(\frac{\pi l}{m}\right)\right]^{-1}\left\{\left[c+b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}-c^{-1/2}\right\}. \tag{B18}$$

with the correction terms

$$R_1=(2m)^{-1}\sum_{l=1}^{m}\left\{\left[t^2+4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}-\left[2b^{1/2}\sin\left(\frac{\pi l}{m}\right)\right]^{-1}\right\}\left\{\left[c+b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}-c^{-1/2}\right\}, \tag{B19}$$

$$R_2=m^{-1}\sum_{l=1}^{m}\left[t^2+4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}\left\{\left[4c+4b\sin^2\left(\frac{\pi l}{m}\right)+t^2\right]^{-1/2}-\left[4c+4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}\right\}. \tag{B20}$$

It is not hard to verify the bounds

$$|R_1|\leqslant(t^2/16b^{1/2}c^{3/2})m^{-1}\sum_{l=1}^{m-1}\csc\left(\frac{\pi l}{m}\right)=O(t^2\ln m), \tag{B21}$$

$$|R_2|\leqslant t/m8c^{3/2}+(t^2/16b^{1/2}c^{3/2})m^{-1}\sum_{l=1}^{m-1}\csc\left(\frac{\pi l}{m}\right)=O\left(\frac{t}{m},t^2\ln m\right). \tag{B22}$$

By removing the leading term the sum I_1^a can be written

$$I_1^a=(2mtc^{1/2})^{-1}+(mc^{1/2})^{-1}\sum_{l=1}^{[m/2]}\left\{\left[t^2+4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}-\left[2b^{1/2}\sin\left(\frac{\pi l}{m}\right)\right]^{-1}\right\}$$
$$+[4m(bc)^{1/2}]^{-1}\sum_{l=1}^{m-1}\csc\left(\frac{\pi l}{m}\right), \tag{B23}$$

where $[x]$ denotes the integer part of x. Ferdinand and Fisher[25] evaluate the last sum as

$$m^{-1}\sum_{l=1}^{m-1}\csc\left(\frac{\pi l}{m}\right)=\left(\frac{2}{\pi}\right)\left\{C_E+\ln\left(\frac{2m}{\pi}\right)\right\}+O(m^{-2}), \tag{B24}$$

where C_E is Euler's constant and the correction term follows by more careful analysis. It is easy to check that we have

$$c^{-1/2}\sum_{l=[m/2]}^{\infty}\{(2b^{1/2}\pi l)^{-1}-[t^2m^2+4b\pi^2l^2]^{-1/2}\}=O(t^2). \tag{B25}$$

Consequently, the sum I_1^a becomes

$$I_1^a=(2mtc^{1/2})^{-1}+[4\pi(bc)^{1/2}]^{-1}\left\{2C_E+2\ln\left(\frac{2m}{\pi}\right)-R_{1/2,0}\left(\frac{t^2m^2}{4b\pi^2}\right)\right\}+R_3+O(t^2), \tag{B26}$$

in which $R_{1/2,0}(x)$ is the remnant function[26] and

$$R_3=(mc^{1/2})^{-1}\sum_{l=1}^{[m/2]}\left\{\left[t^2+4b\sin\left(\frac{\pi l}{m}\right)\right]^{-1/2}-\left[2b^{1/2}\sin\left(\frac{\pi l}{m}\right)\right]^{-1}-\left[t^2+\frac{4b\pi^2l^2}{m^2}\right]^{-1/2}+\left[\frac{2b^{1/2}\pi l}{m}\right]^{-1}\right\}$$
$$\approx-\left[\frac{t^2}{2(2b^{1/2})^3c^{1/2}}\right]m^{-1}\sum_{l=1}^{[m/2]}\left[\csc^3\left(\frac{\pi l}{m}\right)-\left(\frac{m}{\pi l}\right)^3\right]+\left[\frac{3t^4}{8(2b^{1/2})^5c^{1/2}}\right]m^{-1}\sum_{l=1}^{[m/2]}\left[\csc^5\left(\frac{\pi l}{m}\right)-\left(\frac{m}{\pi l}\right)^5\right], \tag{B27}$$

where we have expanded in powers of t^2. We can use the same devices as developed by Ferdinand and Fisher in deriving (B24) to obtain

$$m^{-1}\sum_{l=1}^{[m/2]}\left[\csc^3\left(\frac{\pi l}{m}\right)-\left(\frac{m}{\pi l}\right)^3\right]=\tfrac{1}{2}\pi^{-1}\ln m+O(1), \tag{B28}$$

$$m^{-1}\sum_{l=1}^{[m/2]}\left[\csc^5\left(\frac{\pi l}{m}\right)-\left(\frac{m}{\pi l}\right)^5\right]=O(m^2). \tag{B29}$$

These results show that the correction term R_3 is or order $t^2\ln m$, or t^4m^2. The lemma (B4) can be used[24] to convert the sum I_1^b to an integral plus a correction, namely,

$$I_1^b=\frac{1}{4\pi b^{1/2}}\int_0^{\pi}\frac{d\theta}{\sin\theta}\left([c+b\sin^2\theta]^{-1/2}-c^{-1/2}\right)+R_4=-[4\pi(bc)^{1/2}]^{-1}\ln\left[\frac{b+c}{c}\right]+R_4, \tag{B30}$$

where

$$R_4 = \frac{1}{2\pi b^{1/2}} \sum_{l=1}^{\infty} \int_0^{\pi} \frac{d\theta}{\sin\theta} \cos(2ml\theta)([c+b\sin^2\theta]^{-1/2} - c^{-1/2})$$

$$= \frac{1}{2\pi b^{1/2}} \sum_{l=1}^{\infty} \int_0^{\pi} d\theta \cos(2ml\theta)\left[-\frac{1}{2}\frac{b}{c^{3/2}}\sin\theta + O(\sin^3\theta)\right]. \qquad \text{(B31)}$$

Since

$$\int_0^{\pi} \cos 2p\theta \sin\theta \, d\theta = \frac{2}{1-4p^2} \approx \frac{1}{2p^2}, \quad \int_0^{\pi} \cos 2p\theta \sin^{2k+1}\theta \, d\theta = O(p^{-2k-2}), \qquad \text{(B32)}$$

we conclude that R_4 is of the order m^{-2}. On combining (B26) and (B30), we establish the result

$$I_1 = (2mtc^{1/2})^{-1} + [4\pi(bc)^{1/2}]^{-1}\left\{2C_E + 2\ln\left(\frac{2m}{\pi}\right) - R_{1/2,0}\left(\frac{t^2m^2}{4b\pi^2}\right) - \ln\left[\frac{b+c}{c}\right]\right\} + O(t^2\ln m, m^{-2}). \qquad \text{(B33)}$$

Now we write

$$I_1 - I_2 = 2\sum_{l=1}^{m} \sin^2\left(\frac{\pi l}{m}\right)\Big/ X\left(\frac{2\pi l}{m}\right) = (2mb^{1/2})^{-1}\sum_{l=1}^{m}\sin\left(\frac{\pi l}{m}\right)\left[c + b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2} + R_5 + R_6 + R_7, \qquad \text{(B34)}$$

where the correction terms, whose order of magnitude can be easily estimated, are

$$R_5 = -\frac{t^2}{2bm}\sum_{l=1}^{m-1}\left[t^2 + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}\left[4c + 4b\sin^2\left(\frac{\pi l}{m}\right) + t^2\right]^{-1/2} = O(t^2\ln m), \qquad \text{(B35)}$$

$$R_6 = (2bm)^{-1}\sum_{l=1}^{m-1}\left[4c + 4b\sin^2\left(\frac{\pi l}{m}\right) + t^2\right]^{-1/2}\left\{\left[t^2 + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{1/2} - 2b^{1/2}\sin\left(\frac{\pi l}{m}\right)\right\} = O(t^2\ln m), \qquad \text{(B36)}$$

$$R_7 = (mb^{1/2})^{-1}\sum_{l=1}^{m-1}\sin\left(\frac{\pi l}{m}\right)\left\{\left[4c + 4b\sin^2\left(\frac{\pi l}{m}\right) + t^2\right]^{-1/2} - \left[4c + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}\right\} = O(t^2). \qquad \text{(B37)}$$

In analogy to (B30) and (B31), we find the sum in (B34) can be written as sums of integrals or as the sums of certain Fourier coefficients of the summand,

$$I_1 - I_2 = \frac{1}{2\pi b^{1/2}}\int_0^{\pi}\frac{d\theta\sin\theta}{[c+b\sin^2\theta]^{1/2}} + \frac{1}{\pi b^{1/2}}\sum_{l=1}^{\infty}\int_0^{\pi} d\theta\,\frac{\cos(2ml\theta)\sin\theta}{|c|^{1/2}} + O(m^{-4}, t^2\ln m)$$

$$= \frac{1}{\pi b}\tan^{-1}\left(\frac{b}{c}\right)^{1/2} - \frac{\zeta(2)}{2\pi(bc)^{1/2}}\,\frac{1}{m^2} + O(t^2\ln m, m^{-4}), \qquad \text{(B38)}$$

where $\zeta(2) = \frac{1}{6}\pi^2$ is the Riemann ζ function.

Finally, we obtain

$$I_1 - 2I_2 + I_3 = 4\sum_{l=1}^{m}\sin^4\left(\frac{\pi l}{m}\right)\Big/ X\left(\frac{2\pi l}{m}\right) = (b^{1/2}m)^{-1}\sum_{l=1}^{m-1}\sin^3\left(\frac{\pi l}{m}\right)\Big/\left[c + b\sin^2\left(\frac{\pi l}{m}\right)\right]^{1/2} + R_8 + R_9 + R_{10}, \qquad \text{(B39)}$$

in which the correction terms are

$$R_8 = -\frac{t^2}{bm}\sum_{l=1}^{m-1}\sin^2\left(\frac{\pi l}{m}\right)\left[t^2 + 4c + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}\left[t^2 + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2} = O(t^2), \qquad \text{(B40)}$$

$$R_9 = (bm)^{-1}\sum_{l=1}^{m-1}\sin^2\left(\frac{\pi l}{m}\right)\left[t^2 + 4c + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}\left\{\left[t^2 + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{1/2} - 2b^{1/2}\sin\left(\frac{\pi l}{m}\right)\right\} = O(t^2), \qquad \text{(B41)}$$

$$R_{10} = \frac{2}{b^{1/2}m}\sum_{l=1}^{m-1}\sin^3\left(\frac{\pi l}{m}\right)\left\{\left[t^2 + 4c + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2} - \left[4c + 4b\sin^2\left(\frac{\pi l}{m}\right)\right]^{-1/2}\right\} = O(t^2). \qquad \text{(B42)}$$

On using (B4) and (B32), the sum in (B39) becomes an integral so that we obtain

$$I_1 - 2I_2 + I_3 = \frac{1}{\pi b^{1/2}} \int_0^\pi \frac{d\theta \sin^3\theta}{[c + b\sin^2\theta]^{1/2}} + O(m^{-4}) + R_8 + R_9 + R_{10},$$

$$= \frac{b-c}{\pi b^2} \tan^{-1}\left(\frac{b}{c}\right)^{1/2} + \frac{c^{1/2}}{\pi b^{3/2}} + O(t^2, m^{-4}). \qquad \text{(B43)}$$

This completes the calculation of I_1, I_2, and I_3.

Sums J_i

We shall first show that the denominator $Y(\theta)$ in these sums is exponentially small for θ away from the origin; hence the main contribution comes from the region where θ is small. It is easily verified using the form (B45) that the term inside the braces in $Y(\theta)$ as given by (B8) satisfies the inequality

$$[a - 2b\cos\theta]/2c + X(\theta)/2c \geq 1. \qquad \text{(B44)}$$

Since $\cos\theta$ is a decreasing function of θ for $0 \leq \theta \leq \frac{1}{2}\pi$, we find that $X(\theta)$, and hence the above expression and $Y(\theta)$, are increasing functions of θ. Therefore for $[\frac{1}{2}m] \geq l \geq l_c$, we have

$$Y\left(\frac{2\pi l}{m}\right) \geq Y\left(\frac{2\pi l_c}{m}\right) = \left\{1 + \frac{[t^2 + 4b\sin^2(\pi l_c/m)]}{2c} + \frac{X(2\pi l_c/m)}{2c}\right\}^n - 1$$

$$\geq \left\{1 + 2\left(\frac{b}{c}\right)^{1/2} \sin\left(\frac{\pi l_c}{m}\right)\right\}^n - 1 \approx \exp\left[2\pi l_c \left(\frac{b}{c}\right)^{1/2} \frac{n}{m}\right] - 1, \qquad \text{(B45)}$$

for $l_c \ll m$. If we choose l_c such that $1 \ll l_c \ll m$, then $Y(2\pi l/m)^{-1}$ is exponentially small for $l \geq l_c$. Consequently, we can write

$$J_1 = [mX(0)Y(0)]^{-1} + \frac{2}{m} \sum_{l=1}^{l_c} \left[X\left(\frac{2\pi l}{m}\right) Y\left(\frac{2\pi l}{m}\right)\right]^{-1} + O(e^{-Ql_c}), \qquad \text{(B46)}$$

where Q is a positive constant. In the interval $0 \leq \theta \leq 2\pi l_c/m \ll 1$, we expand $Y(\theta)^{-1}$ and $X(\theta)^{-1}$ around the origin to obtain

$$\frac{1}{Y(2\pi l/m)} \approx \left(e^{\bar{n}W/\bar{m}} - 1\right)^{-1} + \left(\cosh\left[\frac{\bar{n}W}{\bar{m}}\right] - 1\right)^{-1} \left[\frac{\frac{1}{48}\bar{n}W^3}{\bar{m}^3 c} - \frac{\frac{1}{3}(\pi l)^4 \bar{n}}{b\bar{m}^3 W}\right] + \cdots, \qquad \text{(B47)}$$

$$\frac{1}{mX(2\pi l/m)} \approx [2(cb)^{1/2} W]^{-1} \left[1 + \frac{\frac{2}{3}(\pi l)^4}{\bar{m}^2 b W^2} - \frac{W^2}{8\bar{m}^2 c} + \cdots\right], \qquad \text{(B48)}$$

where

$$\bar{n} = \frac{n}{c^{1/2}}, \quad \bar{m} = \frac{m}{b^{1/2}}, \quad \text{and} \quad W = W(l) = [t^2 \bar{m}^2 + 4\pi^2 l^2]^{1/2}. \qquad \text{(B49)}$$

In particular, for $l = 0$ we have $W(0) = |t|\bar{m}$ and

$$[mX(0)Y(0)]^{-1} = [2c^{1/2} m|t|]^{-1} [e^{\bar{n}|t|} - 1]^{-1} \{1 + O(t^2)\}. \qquad \text{(B50)}$$

These results give

$$J_1 = [2c^{1/2} m|t|]^{-1} [e^{\bar{n}|t|} - 1]^{-1} + (bc)^{-1/2} \sum_{l=1}^{\infty} 1/W(l)[e^{\bar{n}W(l)/\bar{m}} - 1] + R_{11}, \qquad \text{(B51)}$$

with correction term

$$R_{11} = (bc)^{-1/2} \sum_{l=1}^{\infty} \left\{[e^{\bar{n}W(l)/\bar{m}} - 1]^{-1} \left[\frac{\frac{2}{3}(\pi l)^4}{\bar{m}^2 b W^3} - \frac{W}{8\bar{m}^2 c}\right]\right.$$

$$\left. + \left[\cosh\left(\frac{\bar{n}W}{\bar{m}}\right) - 1\right]^{-1} \left[\frac{\bar{n}W^3}{48\bar{m}^3 c} - \frac{(\pi l)^4 \bar{n}}{3b\bar{m}^3 W}\right]\right\} + O(e^{-Ql_c}). \qquad \text{(B52)}$$

Since the two series

$$\sum_{l=1}^{\infty} \frac{W(l)}{e^{\bar{n}W(l)/\bar{m}} - 1}, \quad \sum_{l=1}^{\infty} \frac{W(l)^3}{\cosh[\bar{n}W(l)/\bar{m}] - 1} \qquad \text{(B53)}$$

converge, the correction term R_{11} is of the order m^{-2}.

Since we can write

$$J_1 - J_2 = \frac{2}{m} \sum_{l=1}^{m-1} \sin^2\left(\frac{\pi l}{m}\right) \Big/ X\left(\frac{2\pi l}{m}\right) Y\left(\frac{2\pi l}{m}\right), \tag{B54}$$

the results (B45), (B47), and (B48) may be used to give

$$J_1 - J_2 = \tfrac{1}{2} m^{-2} (bc)^{-1/2} \sum_{l=1}^{\infty} \frac{(2\pi l)^2}{W(l)[e^{\bar{n} W(l)/\bar{m}} - 1]} + O(m^{-4}, e^{-Q l_c}). \tag{B55}$$

The above sum may be approximated by its value at $T = T_c$ ($t = 0$), and we find

$$J_1 - J_2 = \tfrac{1}{2} m^{-2} (bc)^{-1/2} \sum_{l=1}^{\infty} \frac{2\pi l}{e^{2\pi l \bar{n}/\bar{m}} - 1} + O(t^2, m^{-4}, e^{-Q l_c}). \tag{B56}$$

Likewise we obtain

$$J_1 - 2J_2 + J_3 = \frac{4}{m} \sum_{l=1}^{m-1} \sin^4\left(\frac{\pi l}{m}\right) \Big/ X\left(\frac{2\pi l}{m}\right) Y\left(\frac{2\pi l}{m}\right) = O(m^{-4}). \tag{B57}$$

These results for I_j and J_j can be used to evaluate the double sums $S_{pq}(m, n)$.

Double sum $S_{00}(n,m)$

From (B7), (B13), and (B14), we have

$$S_{00}(n, m) = I_1 + 2J_1, \tag{B58}$$

and on substituting the result (B33) for I_1 and (B51) for J_1, we find

$$S_{00}(n,m) = [c^{1/2} m|t|]^{-1}\left(\tfrac{1}{2} + \frac{1}{e^{\bar{n}|t|} - 1}\right) + [4\pi(bc)^{1/2}]^{-1}\left\{2C_E + 2\ln\left(\frac{2m}{\pi}\right) - R_{1/2,0}\left(\frac{\bar{m}^2 t^2}{4\pi^2}\right) - \ln\left(\frac{b+c}{c}\right) + 8\pi \sum_{l=1}^{\infty} 1/W(l)[e^{W(l)\bar{n}/\bar{m}} - 1]\right\}. \tag{B59}$$

It can be seen from the definition of S_{00} that this double sum is invariant under the transformation $m \rightarrow n$, $b \rightarrow c$. We shall check that this property is indeed satisfied by our expression for S_{00}. The function $(e^x - 1)^{-1}$ has the expansion in simple fractions[27]

$$(e^x - 1)^{-1} = x^{-1} - \tfrac{1}{2} + 2x \sum_{k=1}^{\infty} (x^2 + 4\pi^2 k^2)^{-1}. \tag{B60}$$

From this we find

$$\begin{aligned} &\sum_{l=1}^{\infty} \{W(l)^{-1}[e^{W(l)\bar{n}/\bar{m}} - 1]^{-1} - (2\pi l)^{-1}[e^{2\pi l \bar{n}/\bar{m}} - 1]^{-1}\} \\ &= \frac{1}{2|t|\bar{n}}\left[\tfrac{1}{2}\coth(\tfrac{1}{2}|t|\bar{m}) - \frac{1}{|t|\bar{m}} - \tfrac{1}{12}|t|\bar{m}\right] + \frac{1}{8\pi} R_{1/2,0}\left(\frac{t^2 \bar{m}^2}{4\pi^2}\right) \\ &+ 2\sum_{l=1}^{\infty}\sum_{k=1}^{\infty}\left[\left(t^2 mn + \frac{4\bar{m}\pi^2 l^2}{\bar{n}} + \frac{4\bar{n}\pi^2 k^2}{\bar{m}}\right)^{-1} - \left(\frac{4\bar{m}\pi^2 l^2}{\bar{n}} + \frac{4\bar{n}\pi^2 k^2}{\bar{m}}\right)^{-1}\right]. \end{aligned} \tag{B61}$$

Now let us put

$$F(\tau) = \sum_{l=1}^{\infty} \frac{1}{l(e^{2\pi l \tau} - 1)} + \frac{\pi\tau}{12}. \tag{B62}$$

On substituting these two relations into the last term of (B59), we may express S_{00} as

$$S_{00} = \frac{1}{t^2 mn} + \frac{1}{2\pi(bc)^{1/2}}[\ln(mn)^{1/2} + P(\bar{m}t, \bar{n}t)] + O(m^{-2}, t^2 \ln m), \tag{B63}$$

where

$$\begin{aligned} P(x,y) = {} & \pi x^{-1}[\coth\tfrac{1}{2}y - 2y^{-1} - \tfrac{1}{6}y] + \pi y^{-1}[\coth\tfrac{1}{2}x - 2x^{-1} - \tfrac{1}{6}x] + C_E + \ln\left(\frac{2}{\pi}\right) - \tfrac{1}{4}\ln\left[\frac{(b+c)^2}{bc}\right] + \tfrac{1}{2}\ln\left(\frac{x}{y}\right) + 2F\left(\frac{y}{x}\right) \\ & + 8\pi\sum_{l=1}^{\infty}\sum_{k=1}^{\infty}\left(\left[xy + \frac{x}{y}4\pi^2 l^2 + \frac{y}{x}4\pi^2 k^2\right]^{-1} - \left[\left(\frac{x}{y}\right)4\pi^2 l^2 + \left(\frac{y}{x}\right)4\pi^2 k^2\right]^{-1}\right). \end{aligned} \tag{B64}$$

We may now rewrite (B62) as

$$F(\tau)-\tfrac{1}{12}\pi\tau=\sum_{l=1}^{\infty} l^{-1}\sum_{r=1}^{\infty} e^{-2\pi\tau l r}=-\ln\left[\prod_{r=1}^{\infty}(1-e^{-2\pi\tau r})\right]. \tag{B65}$$

Since the elliptic θ functions $\theta_i(v|i\tau)$ satisfy the relation[28]

$$\frac{\theta_2(0|i\tau)\,\theta_3(0|i\tau)\,\theta_4(0|i\tau)}{2e^{-\pi\tau/4}}=\left(\prod_{r=1}^{\infty}(1-e^{-2\pi\tau r})\right)^3, \tag{B66}$$

we have

$$F(\tau)=\tfrac{1}{3}\ln 2-\tfrac{1}{3}\ln[\theta_2(0|i\tau)\,\theta_3(0|i\tau)\,\theta_4(0|i\tau)]. \tag{B67}$$

On using the θ-function identity[29]

$$\theta_i(0|i\tau)=\tau^{-1/2}\theta_i(0|i\tau^{-1}), \tag{B68}$$

we hence find

$$F(\tau)=F(\tau^{-1})+\tfrac{1}{2}\ln\tau. \tag{B69}$$

Therefore we also have

$$2F\left(\frac{y}{x}\right)+\tfrac{1}{2}\ln\left(\frac{x}{y}\right)=2F\left(\frac{x}{y}\right)+\tfrac{1}{2}\ln\left(\frac{y}{x}\right). \tag{B70}$$

This establishes that $P(x,y)=P(y,x)$ and that S_{00} is symmetric in $\overline{m}$, $\overline{n}$ as required.

Sums S_{01}, S_{10}, S_{11}

The sum S_{01}, given by (B9), can be written

$$S_{10}=S_{00}-(I_1-I_2)-2(J_1-J_2). \tag{B71}$$

Hence (B38) and (B56) yield

$$S_{10}=S_{00}-\frac{1}{\pi b}\tan^{-1}\left(\frac{b}{c}\right)^{1/2}+(bc)^{1/2}\frac{G(\tau)}{m^2}+O(t^2\ln m, m^{-4}), \tag{B72}$$

where $\tau=\overline{n}/\overline{m}$ and

$$G(\tau)=\frac{\zeta(2)}{2\pi}+\sum_{l=1}^{\infty}\frac{2\pi l}{e^{2\pi l\tau}-1}. \tag{B73}$$

It is not difficult to see

$$G(\tau)=\frac{\pi}{12}-\frac{d}{d\tau}\sum_{l=1}^{\infty}\ln(1-e^{-2\pi l\tau})=\frac{d}{d\tau}F(\tau). \tag{B74}$$

Thus we may differentiate both sides of (B69) to obtain the relation

$$\tau G(\tau)+\tau^{-1}G(\tau^{-1})=\tfrac{1}{2}. \tag{B75}$$

From (B11) we then find

$$S_{01}=-(2c)^{-1}+\left[\frac{a-2b}{2c}\right]S_{00}+\left(\frac{b}{c}\right)\left[\frac{1}{\pi b}\tan^{-1}\left(\frac{b}{c}\right)^{1/2}-(bc)^{-1/2}\frac{G(\tau)}{m^2}\right]+O(t^2\ln m, m^{-4}). \tag{B76}$$

Because

$$\tan^{-1}(b/c)^{1/2}=\tfrac{1}{2}\pi-\tan^{-1}(c/b)^{1/2} \tag{B77}$$

and

$$[(a-2b)/2c]S_{00}=S_{00}+t^2S_{00}/2c=S_{00}+(2cmn)^{-1}+O(t^2\ln m) \tag{B78}$$

[in which we have used (B63)], we can write S_{01} in the form

$$S_{01}=S_{00}-(1/\pi c)\tan^{-1}(c/b)^{1/2}+(cmn)^{-1}[\tfrac{1}{2}-\tau G(\tau)]+O(t^2\ln m, m^{-4}). \tag{B79}$$

On using the identity (B75) for $G(\tau)$, we obtain

$$S_{01}=S_{00}-\frac{1}{\pi c}\tan^{-1}\left(\frac{c}{b}\right)^{1/2}+(bc)^{1/2}\frac{G(\tau^{-1})}{n^2}+O(t^2\ln m, m^{-4}). \tag{B80}$$

Finally, we can write S_{11}, given by (B12), as

$$S_{11}=\left[\frac{a-4b}{2c}\right]S_{10}+\left(\frac{b}{c}\right)S_{00}-\left(\frac{b}{c}\right)[(I_3+I_1-2I_2)+2(J_3+J_1-2J_2)]. \tag{B81}$$

The results (B43), (B57), and (B80) yield

$$S_{11}=\left[\frac{a-2b}{2c}\right]S_{00}-\frac{t^2}{2\pi bc}\tan^{-1}\left(\frac{b}{c}\right)^{1/2}-\frac{1}{\pi(bc)^{1/2}}+\left[\frac{a-4b}{2c}\right](bc)^{-1/2}\frac{G(\tau)}{m^2}+O(t^2\ln m, m^{-4}). \tag{B82}$$

On using (B78) and (3.18) we find

$$S_{11}=S_{00}+(2cmn)^{-1}-\frac{1}{\pi(bc)^{1/2}}-\left[\frac{b}{c}-1\right](bc)^{-1/2}\frac{G(\tau)}{m^2}+O(t^2\ln m, m^{-4}). \tag{B83}$$

Thus the identity (B75) yields

$$S_{11}=S_{00}-\frac{1}{\pi(bc)^{1/2}}+(bc)^{-1/2}\frac{G(\tau)}{m^2}+(bc)^{-1/2}\frac{G(\tau^{-1})}{n^2}+O(t^2\ln m,m^{-4}), \qquad (B84)$$

where we recall that $G(\tau)$ is defined through (B74) and (B67) in terms of elliptic θ functions.

APPENDIX C: CORRECTION TERM

In the limit $n,m\to\infty$, the total defect free energy (2.26) behaves as the bulk free energy plus the incremental free energy $f_1(T)$ due to a single isolated defect, except for the correction term

$$e(T)=f(T)-f_0(T)-(nm)^{-1}f_1(T), \qquad (C1)$$

which will be shown to be of the order $e^{-\sigma m/\xi_1}$ or $e^{-\sigma n/\xi_2}$, where $\xi_1(T)$ and $\xi_2(T)$ are the bulk correlation lengths in the vertical and horizontal directions,[30] respectively, while $\sigma=2$ for $T>T_c$ but $\sigma=1$ for $T<T_c$. The correlation lengths may, as usual, be defined in terms of the asymptotic decay of the pair correlations above T_c according to

$$\langle s_{00}s_{0m}\rangle\sim\exp[-m/\xi_1(T)],\qquad \langle s_{00}s_{n0}\rangle\sim\exp[-n/\xi_2(T)], \qquad (C2)$$

as $m,n\to\infty$. For simplicity, we will consider explicitly only single-bond defects [see Fig. 2(b)]; however, from our calculation, one can see that the result is true for all defects.

From (4.1) we find the error to be

$$e(T)=\frac{1}{2mn}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_2}{2\pi}\ln|\underline{y}_b^{-1}+\underline{G}_b|-\frac{1}{nm}|[0,1]_{RL}^{\infty}-(z_1'-z_1)^{-1}|, \qquad (C3)$$

where the 2×2 determinant is given by

$$|\underline{y}_b^{-1}+\underline{G}_b|=[0,0]_{RR}[0,0]_{LL}-\{[0,1]_{RL}-(z_1'-z_1)^{-1}\}\{[0,-1]_{LR}+(z_1'-z_1)^{-1}\}, \qquad (C4)$$

in which the elements $[l,k]_{\lambda\mu}$ are given by (2.25). Let us define the double sums

$$R_{p,q}(m,n)=\frac{1}{nm}\sum_{\phi_1}\sum_{\phi_2}\frac{e^{-ip\phi_1-ip\phi_2}}{\Delta(\phi_1,\phi_2)}, \qquad (C5)$$

where $\Delta(\phi_1,\phi_2)$ is given by (2.19), while ϕ_1 and ϕ_2 run over the m,n values specified in (2.18). We can then express the matrix elements $[l,k]_{\lambda\mu}$ as linear combination of the sums $R_{p,q}$. By generalizing the lemma of Barber and Fisher[24] we can reexpress these sums in the form

$$R_{p,q}=\sum_{j=-\infty}^{\infty}\sum_{j'=-\infty}^{\infty}A_{p+jm,q+j'n}e^{i(j\theta_1+j'\theta_2)}, \qquad (C6)$$

where $A_{r,s}$ are the Fourier coefficients of $1/\Delta(\phi_1,\phi_2)$ as defined by (3.3). The leading coefficient $A_{p,q}$ clearly corresponds to the integral approximation to $R_{p,q}(m,n)$ valid as $m,n\to\infty$. One of the integrations defining $A_{r,s}$ can now be carried out explicitly to yield[31]

$$A_{r,s}=\int_0^{2\pi}\frac{d\theta}{2\pi}\frac{\cos r\theta}{X(\theta)}\times\left(\frac{[a-2b\cos\theta+X(\theta)]}{2c}\right)^{-|s|}, \qquad (C7)$$

in which $X(\theta)$ is defined by (B7).

Since $X(\theta)$ is analytic in the strip $0<|\theta|<\theta_c$, where

$$\theta_c=2\sinh|t|/2b^{1/2}\approx|t|/b^{1/2}, \qquad (C8)$$

we can use the argument of Barber and Fisher[24] to show that $A_{r,0}$ is exponentially small in r, namely,

$$A_{r,0}=O[\exp(-|rt|/b^{1/2})]. \qquad (C9)$$

On comparing the integrand of (C7) with (B8), (B45), and (B15), we can establish the bound

$$\left(\frac{[a-2b\cos\theta+X(\theta)]}{2c}\right)^{-|s|}\leqslant\left(1+\frac{|t|}{c^{1/2}}\right)^{-|s|}\approx\exp\left(\frac{-|st|}{c^{1/2}}\right). \qquad (C10)$$

In combination with (C9), this yields the basic estimate

$$A_{r,s}=O[\exp(-|rt|/b^{1/2}-|st|/c^{1/2})]. \qquad (C11)$$

Therefore in leading order as $m,n\to\infty$ we have

$$R_{p,q}(m,n)=A_{p,q}+\sum_{j=\pm1}(A_{jm+p,q}e^{ij\theta_1}+A_{p,jn+q}e^{ij\theta_2})+\cdots, \qquad (C12)$$

where the form of the remaining terms is easy to see but will not, in fact, effect the final result.

Now we may substitute (C12) into (C4), using the appropriate linear combinations to express $[0,0]_{RR}$, etc., and hence into (C3). The logarithm in (C3) may then be expanded for $T\neq T_c$ in powers of $A_{\pm m,0}$, $A_{0,\pm n}$, $A_{\pm m+1,0}$, etc., to yield a Fourier series. Integration over θ_1 and θ_2 is trivial for the terms independent of m and n which then cancel exactly in (C4). The only nonvanishing contributions come from products of the form $A_{m,0}A_{-m,0}$, $A_{0,n}A_{0,-n}$, etc., which are at least quadratic in the $A_{m,0}$, etc. Thus by the estimate (C11) the error term $e(T)$ is of order $\exp(-2m|t|/b^{1/2})$ or $\exp(-2n|t|/c^{1/2})$ for $t\neq0$. This confirms our statement.

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[22]The equality $C_1 = C_0^2$ and the simple form of the $x^3 \ln^2 x$ term in (5.1) are not predicted by scaling. (In the notation of Ref. 13 it amounts to the "coincidence" $b/a = \frac{1}{2} A_0$.) Indeed, even though valid for all the defect types studied, the significance and generality of these results remains obscure to us. Some insight may be gained through the following observation: The result (5.1) is implied by the (postulated) critical-point equation $u_0 t + f_{\text{sing}}(t) \approx -D_1 x - D_2(\tau) x^2 + \cdots$ (where $f_{\text{sing}} = \frac{1}{2} A_0 t^2 \ln|t|^{-1}$ is the singular part of the free energy per site) *provided* that $D_1 \equiv 1$ and $u_0 = A_0/C_0$ [while $D_2(\tau)$ must be related to $Q_3(\tau)$]. The values of Q_1 and Q_2 can be regarded as merely fixing D_1 and u_0 as stated (although the result for D_1 is most suggestive); however, the correctly predicted value of Q_4 provides a nontrivial check on the proposed critical equation.
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