

## Exact solutions for even-number correlations of the square Ising model

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To obtain an unusually large set of exact solutions for even-number localized correlations of the standard square Ising model, a method is developed that combines traditional Pfaffian techniques with linear-algebraic systems of correlation identities having interaction-dependent coefficients. Two eight-site clusters (subclusters of the "Greek cross" cluster) are studied, and altogether *sixty* different even-number correlations are determined exactly at all temperatures. Besides demonstrating the existence of degeneracies within the set of exact solutions, the solution curve for an eight-site correlation is evidently the first of such large order to be displayed for an Ising model on any regular planar lattice. Significant time as well as labor efficiency of the method is clearly demonstrated since relatively few correlations need to be actually calculated by Pfaffian techniques in order to obtain large additional numbers of multisite correlation solutions using much simpler linear-algebraic procedures.

### I. INTRODUCTION

Of all the models in statistical mechanics on which exact calculations have been performed, the two-dimensional Ising model is the most investigated.<sup>1</sup> The model was originally introduced as one for ferromagnetism, but later was applied with even more success to binary alloys,<sup>2</sup> and subsequently to "lattice gases,"<sup>3</sup> ferroelectric crystals, DNA,<sup>4</sup> and many other physical systems. A quantitative statement about the existence of a phase transition in the two-dimensional model was first given in 1941 by Kramers and Wannier,<sup>5</sup> and Montroll.<sup>6</sup> The most remarkable development was made in 1944 by Onsager<sup>7</sup> who was able to compute the free energy and "boundary tension" of the Ising model on the square lattice in the absence of magnetic field, and the spin correlation was first derived in 1949 by Kaufman and Onsager.<sup>8</sup> The spontaneous magnetization was announced without derivation by Onsager in 1949, and a derivation was published in 1952 by Yang.<sup>9</sup> The methods of Onsager, Kaufman, and Yang are very complicated but by the 1960's, through the efforts of many researchers, the analyses became more tractable and, since then, these and other methods are actively being used for computing many more quantities of physical interest.

The study of correlation behaviors among the various degrees of freedom comprising an interacting many-body system in thermodynamic equilibrium has leading importance for the basic understanding of the cooperative effects exhibited by such systems. Since correlations are the thermal expectation values of the product of spin variables, they offer a more detailed description than thermodynamic for the order and symmetry present in the system. It is well known from statistical-mechanical fluctuation theory that certain thermodynamic observables, like spontaneous magnetization, magnetic susceptibility and specific heat, to mention a few, can conveniently be represented in terms of correlations. There are

varieties of problems where localized correlations can be utilized e.g., exact analyses of local magnetizations and correlations in the vicinity of an isolated defect perturbing an otherwise isotropic Ising system,<sup>10</sup> in the theory of various transport coefficients as that of superionic conductivity in solid electrolytes like the layered crystalline compound  $\text{AgCrS}_2$ ,<sup>11</sup> to find local magnetic field probability distributions<sup>12</sup> that, in turn, can be used for calculating the inelastic neutron-scattering cross section as well as thermodynamic quantities, and to calculate joint configurational probabilities of Ising variables with use, e.g., in percolation theory, and indeed many other examples of application.

Planar Ising-model even-number multispin correlations have traditionally been calculated by Pfaffian techniques<sup>13</sup> giving exact and explicit solutions. The connection between the Ising problem and Pfaffians was first noticed by Hurst and Green, and then Kasteleyn,<sup>13</sup> in showing the correspondence between Ising and dimer problems, expressed the partition function in terms of a Pfaffian. McCoy, Tracy, and Wu<sup>14</sup> have obtained exact integral-form solutions for arbitrary  $n$ -site Ising correlations on the square lattice, where their expressions are more useful for studying large-distance behaviors of correlations rather than the short-distance behaviors of localized correlations. Various correlations of the square Ising model have more recently been calculated by several authors such as Au-Yang and Perk, Ghosh and Shrock, and Yamada.<sup>15</sup> More specifically, Au-Yang and Perk used quadratic difference equations of Hirota's Toda lattice form to conveniently obtain exact values for the pair correlations at the critical temperature, Ghosh and Shrock developed and analyzed exact and explicit solutions for diagonal, row, and off-axis spin-spin correlations in terms of elliptic integrals, and Yamada expressed the pair correlation in a simple determinantal form called a "generalized Wronskian."

The present paper considers a spin- $\frac{1}{2}$  Ising-model fer-

romagnet having only nearest-neighbor couplings on a square lattice and in zero magnetic field. Exact solutions are obtained for select even-number correlations associated with spatially compact clusters of lattice sites, i.e., where relative distances between sites of the cluster are of the same order of magnitude as the lattice spacing. In this paper, we attempt to develop a comprehensive plan to more efficiently obtain the exact solutions for large numbers of even-number multispin correlations. Two different methods are combined in the present calculations: the Pfaffian techniques and linear-algebraic systems of correlation identities having interaction-dependent coefficients.<sup>16</sup> In Sec. II we define the basic generating equation for the linear-algebraic correlation identities, and in Sec. III the even-number-correlations calculations and results are discussed in detail. Finally, in Sec. IV we summarize and make comments about the analysis and results.

## II. THE SQUARE ISING MODEL AND THE BASIC GENERATING EQUATION FOR ITS LINEAR-ALGEBRAIC CORRELATION IDENTITIES

Consider a lattice consisting of  $N$  sites labeled  $j=0, 1, \dots, N-1$ . At each site there is an atom or ion possessing a magnetic moment (spin) which can only point in two directions, "up" (+) or "down" (-). The two possible cases are described by a state variable, denoted by  $\sigma_j$  for the spin at the site  $j$ , which is +1 for an "up" spin and -1 for a "down" spin. The states of the whole system are, therefore, described by all possible realizations of the set of Ising variables  $\{\sigma_0, \sigma_1, \dots, \sigma_{N-1}\}$ . The Hamiltonian of the Ising model is defined by

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad (2.1)$$

where  $\sum_{\langle i,j \rangle} \dots$  designates summation over all distinct nearest-neighbor pairs of lattice sites, and  $J$ , the interaction parameter, is a positive (negative) quantity for a ferromagnetic (antiferromagnetic) system. The magnetic canonical partition function  $Z$  is given by the usual trace formula over all degrees of freedom of the system

$$Z = \text{Tr}_{\sigma_0, \sigma_1, \dots, \sigma_{N-1}} e^{-\beta H}, \quad (2.2)$$

where  $\beta \equiv 1/k_B T$ ,  $k_B$  being the Boltzmann constant and  $T$  the absolute temperature. Let  $[f]$  be any function of the Ising variables *excluding* the origin-site variable  $\sigma_0$ . One then constructs the canonical thermal average  $\langle \sigma_0 [f] \rangle$  as

$$\begin{aligned} \langle \sigma_0 [f] \rangle &= \frac{1}{Z} \text{Tr}_{\sigma_0, \sigma_1, \dots, \sigma_{N-1}} e^{-\beta H} \sigma_0 [f] \\ &= \left\langle [f] \frac{\text{Tr}_{\sigma_0=\pm 1} e^{\beta J \sigma_0 (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)} \sigma_0}{\text{Tr}_{\sigma_0=\pm 1} e^{\beta J \sigma_0 (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)}} \right\rangle, \end{aligned} \quad (2.3)$$

where the final expression (2.3) has been obtained after some algebraic and partial-trace manipulations, and

where the definition of thermal average has been used (see Fig. 1 for enumeration of lattice sites). Within the thermal average symbol, one may write

$$\begin{aligned} \frac{\text{Tr}_{\sigma_0=\pm 1} e^{\beta J \sigma_0 (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)} \sigma_0}{\text{Tr}_{\sigma_0=\pm 1} e^{\beta J \sigma_0 (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)}} \\ = \tanh K (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4), \end{aligned} \quad (2.4)$$

where  $K = \beta J$  is the (dimensionless) interaction constant. Since  $\tanh K (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)$  is an odd function of its argument, and any Ising variable  $\sigma_l$  satisfies  $\sigma_l^{2n+1} = \sigma_l$  and  $\sigma_l^{2n} = 1$ ,  $n=0, 1, 2, \dots$ , one can write the last equation (2.4) as

$$\begin{aligned} \tanh K (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) &= A (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) \\ &\quad + B (\sigma_1 \sigma_2 \sigma_3 + \sigma_1 \sigma_2 \sigma_4 \\ &\quad + \sigma_1 \sigma_3 \sigma_4 + \sigma_2 \sigma_3 \sigma_4). \end{aligned} \quad (2.5)$$

The coefficients  $A$  and  $B$  are only dependent on the interaction constant  $K$  and can be evaluated by using all possible values of the Ising variable  $\sigma_1, \sigma_2, \sigma_3, \sigma_4$  in Eq. (2.5), that lead to

$$\begin{aligned} A &= \frac{1}{8} (\tanh 4K + 2 \tanh 2K), \\ B &= \frac{1}{8} (\tanh 4K - 2 \tanh 2K). \end{aligned} \quad (2.6)$$

Substituting (2.4) and (2.5) into (2.3) gives

$$\begin{aligned} \langle \sigma_0 [f] \rangle &= A \langle (\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4) [f] \rangle \\ &\quad + B \langle (\sigma_1 \sigma_2 \sigma_3 + \sigma_1 \sigma_2 \sigma_4 \\ &\quad + \sigma_1 \sigma_3 \sigma_4 + \sigma_2 \sigma_3 \sigma_4) [f] \rangle, \quad \sigma_0 \notin [f], \end{aligned} \quad (2.7)$$

where  $A$  and  $B$  are given by Eq. (2.6). Equation (2.7) is the *basic generating equation* for Ising correlations upon the square lattice and will be used throughout the calcu-

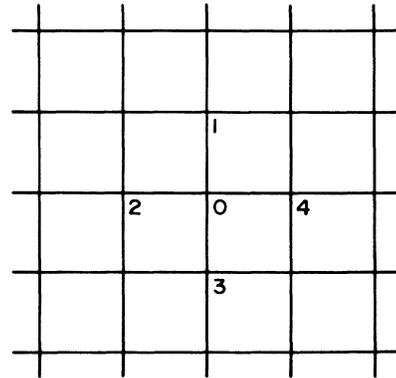
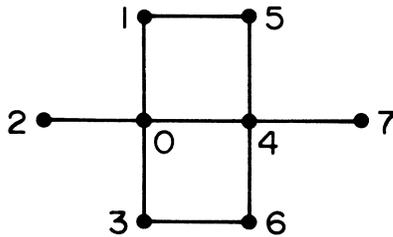


FIG. 1. An elementary cluster of the square lattice, where zero is the origin site and 1, 2, 3, and 4 are its nearest-neighbor sites.

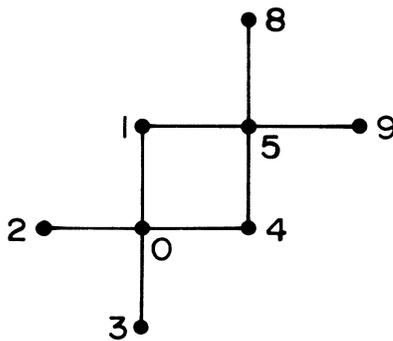
lations to generate the linear-algebraic systems of correlation identities.

### III. EVEN-NUMBER LOCALIZED CORRELATIONS OF THE SQUARE ISING FERROMAGNET

We wish to explore and develop a highly efficient procedure for obtaining the exact solutions for all even-number correlations on a chosen eight-site cluster [see Fig. 2(a)]. Using the rotational, translational, and inversion symmetry, investigation offers 35 nonequivalent correlations exhausting all the possibilities defined upon the eight-site cluster. Five are pair-correlations, eighteen are quartet-correlations, eleven are sextet-correlations, and one is an octet-correlation. Using the basic generating equation (2.7), where  $[f]$  is any product of an odd-number of spins (*not* containing the origin-site spin) and recalling the fact that for any Ising variable  $\sigma_i^2=1$ , and again using the symmetry group operations for the system Hamiltonian, one obtains 34 linear-algebraic identities. The correlations are given in Table I, where the lattice points are enumerated in Fig. 2(a) as 0, 1, . . . , 7, and for notational simplicity, the spin variables within a thermal average symbol are represented by their corresponding site labels. In Table I the underlined thermal averages are those used to generate identities and one observes, therefore, for a particular correlation sometimes more than one identity can be generated. For example, three different identities can be generated for  $x_6$ . The re-



(a)



(b)

FIG. 2. Extended clusters of the square lattice where both eight-site clusters are segments of the "Greek cross" cluster.

sulting linear identities are the following:

$$x_1 = A + A(2x_2 + x_3) + B(2x_2 + x_3 + x_{18}), \quad (3.1)$$

$$x_2 = 2A(x_1 + x_4) + 2B(x_{13} + x_{14}), \quad (3.2)$$

$$x_3 = A(x_1 + 2x_4 + x_5) + B(x_{16} + 2x_{17} + x_{19}), \quad (3.3)$$

$$x_6 = B + A(2x_2 + x_3 + x_{18}) + B(2x_2 + x_3), \quad (3.4)$$

$$x_6 = A(x_3 + 2x_{10} + x_{11}) + B(2x_{20} + x_{23} + x_{33}), \quad (3.5)$$

$$x_6 = A(x_2 + x_7 + x_8 + x_9) + B(x_{20} + x_{21} + x_{22} + x_{31}), \quad (3.6)$$

$$x_7 = A(x_1 + x_4 + x_{13} + x_{14}) + B(x_1 + x_4 + x_{13} + x_{14}), \quad (3.7)$$

$$x_8 = 2A(x_4 + x_{14}) + 2B(x_1 + x_{13}), \quad (3.8)$$

$$x_9 = A(x_4 + x_5 + x_{17} + x_{19}) + B(x_1 + x_4 + x_{16} + x_{17}), \quad (3.9)$$

$$x_{10} = A(x_1 + x_4 + x_{13} + x_{14}) + B(x_1 + x_4 + x_{13} + x_{14}), \quad (3.10)$$

$$x_{10} = A(x_1 + x_4 + x_{16} + x_{17}) + B(x_4 + x_5 + x_{17} + x_{19}), \quad (3.11)$$

$$x_{11} = A(2x_4 + x_{16} + x_{19}) + B(x_1 + x_5 + 2x_{17}), \quad (3.12)$$

$$x_{12} = 2A(x_1 + x_{13}) + 2B(x_4 + x_{14}), \quad (3.13)$$

$$x_{13} = A(x_3 + x_{10} + x_{20} + x_{23}) + B(x_{10} + x_{11} + x_{20} + x_{33}), \quad (3.14)$$

$$x_{13} = A(x_2 + x_7 + x_{20} + x_{21}) + B(x_8 + x_9 + x_{22} + x_{31}), \quad (3.15)$$

$$x_{14} = A(x_2 + x_8 + x_{20} + x_{22}) + B(x_7 + x_9 + x_{21} + x_{31}), \quad (3.16)$$

$$x_{15} = A(x_1 + x_5 + 2x_{17}) + B(2x_4 + x_{16} + x_{19}), \quad (3.17)$$

$$x_{16} = A(x_3 + x_{11} + 2x_{20}) + B(2x_{10} + x_{23} + x_{33}), \quad (3.18)$$

$$x_{17} = A(x_2 + x_9 + x_{21} + x_{22}) + B(x_7 + x_8 + x_{20} + x_{31}), \quad (3.19)$$

$$x_{18} = A(x_6 + 2x_{14} + x_{19}) + B(x_{26} + 2x_{27} + x_{34}), \quad (3.20)$$

$$x_{24} = 2A(x_{13} + x_{14}) + 2B(x_1 + x_4), \quad (3.21)$$

$$x_{24} = A(x_6 + x_{14} + x_{26} + x_{27}) + B(x_{14} + x_{19} + x_{27} + x_{34}), \quad (3.22)$$

$$x_{25} = A(x_{16} + 2x_{17} + x_{19}) + B(x_1 + 2x_4 + x_5), \quad (3.23)$$

$$x_{25} = A(x_6 + x_{19} + 2x_{27}) + B(2x_{14} + x_{26} + x_{34}), \quad (3.24)$$

$$x_{26} = A(2x_{20} + x_{23} + x_{33}) + B(x_3 + 2x_{10} + x_{11}), \quad (3.25)$$

$$x_{27} = A(x_{20} + x_{21} + x_{22} + x_{31}) + B(x_2 + x_7 + x_8 + x_9), \quad (3.26)$$

$$x_{28} = A(x_{10} + x_{11} + x_{20} + x_{33}) + B(x_3 + x_{10} + x_{20} + x_{23}), \quad (3.27)$$

$$x_{28} = A(x_7 + x_8 + x_{20} + x_{31}) + B(x_2 + x_9 + x_{21} + x_{22}), \quad (3.28)$$

$$x_{29} = A(x_7 + x_9 + x_{21} + x_{31}) + B(x_2 + x_8 + x_{20} + x_{22}), \quad (3.29)$$

$$x_{30} = A(x_8 + x_9 + x_{22} + x_{31}) + B(x_2 + x_7 + x_{20} + x_{21}), \quad (3.30)$$

$$x_{31} = A(x_{14} + x_{19} + x_{27} + x_{34}) + B(x_6 + x_{14} + x_{26} + x_{27}), \quad (3.31)$$

$$x_{32} = A(2x_{10} + x_{23} + x_{33}) + B(x_3 + x_{11} + 2x_{20}), \quad (3.32)$$

$$x_{33} = A(2x_{14} + x_{26} + x_{34}) + B(x_6 + x_{19} + 2x_{27}), \quad (3.33)$$

$$x_{35} = A(x_{26} + 2x_{27} + x_{34}) + B(x_6 + 2x_{14} + x_{19}). \quad (3.34)$$

The set of 34 equations (3.1)–(3.34) in 35 unknowns is linear, algebraic, inhomogeneous, and exact. Upon examining the matrix constructed from the coefficients, it is found that among the 34 linear equations, only 28 are linearly independent. Therefore, one needs knowledge of seven correlations<sup>17</sup> to determine solutions for the totality of 35 correlations. For these, one may choose the five pair correlations  $x_1, x_2, x_3, x_4,$  and  $x_5$  together with the two quartet correlations  $x_{12}$  and  $x_{17}$ . Exact solutions of  $x_1$  and  $x_2$  are shown in a paper by Montroll, Potts, and Ward<sup>13</sup> and  $x_4$  by Mahan;<sup>11</sup> all calculated by Pfaffian techniques. The remaining four correlations are also presently calculated by Pfaffian techniques. With the aid of the aforementioned seven solutions, the remaining 28 correlations are then solved by using the coefficient matrix<sup>17</sup> and standard methods of linear algebra. The final results have been checked by calculating the two quartet correlations  $x_{10}$  and  $x_{23}$  independently by Pfaffian techniques for all temperatures.

After the success on the above eight-site cluster, another eight-site cluster has been chosen on the square lattice [see Fig. 2(b)]. This cluster is diagonally extended with respect to the former cluster. Six lattice sites 0, 1, 2, 3, 4,

TABLE I. Definitions of spin correlations upon the eight-site cluster shown in Fig. 2(a) where the underlined correlations are used as generators for correlation identities.

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$x_1 = \langle \underline{01} \rangle, \langle 02 \rangle, \langle 03 \rangle, \langle 04 \rangle, \langle 15 \rangle, \langle 36 \rangle, \langle 45 \rangle, \langle 46 \rangle, \langle 47 \rangle$
$x_2 = \langle \underline{05} \rangle, \langle 06 \rangle, \langle 12 \rangle, \langle 14 \rangle, \langle 23 \rangle, \langle 34 \rangle, \langle 57 \rangle, \langle 67 \rangle$
$x_3 = \langle \underline{07} \rangle, \langle 13 \rangle, \langle 24 \rangle, \langle 56 \rangle$
$x_4 = \langle 16 \rangle, \langle 17 \rangle, \langle 25 \rangle, \langle 26 \rangle, \langle 35 \rangle, \langle 37 \rangle$
$x_5 = \langle 27 \rangle$
$x_6 = \langle \underline{0123} \rangle, \langle 0124 \rangle, \langle 0134 \rangle, \langle 0234 \rangle, \langle \underline{0456} \rangle, \langle \underline{0457} \rangle, \langle 0467 \rangle, \langle 4567 \rangle$
$x_7 = \langle \underline{0125} \rangle, \langle 0146 \rangle, \langle 0236 \rangle, \langle 0345 \rangle, \langle 1457 \rangle, \langle 3467 \rangle$
$x_8 = \langle \underline{0126} \rangle, \langle 0235 \rangle, \langle 1467 \rangle, \langle 3457 \rangle$
$x_9 = \langle \underline{0127} \rangle, \langle 0237 \rangle, \langle 2457 \rangle, \langle 2467 \rangle$
$x_{10} = \langle \underline{0135} \rangle, \langle 0136 \rangle, \langle \underline{0147} \rangle, \langle 0245 \rangle, \langle 0246 \rangle, \langle 0347 \rangle, \langle 1456 \rangle, \langle 3456 \rangle$
$x_{11} = \langle \underline{0137} \rangle, \langle 2456 \rangle$
$x_{12} = \langle \underline{0145} \rangle, \langle 0346 \rangle$
$x_{13} = \langle \underline{0156} \rangle, \langle 0356 \rangle, \langle 1345 \rangle, \langle 1346 \rangle, \langle \underline{0157} \rangle, \langle 0367 \rangle, \langle 1245 \rangle, \langle 2346 \rangle$
$x_{14} = \langle \underline{0167} \rangle, \langle 0357 \rangle, \langle 1246 \rangle, \langle 2345 \rangle, \langle 1235 \rangle, \langle 1236 \rangle, \langle 1567 \rangle, \langle 3567 \rangle$
$x_{15} = \langle \underline{0247} \rangle$
$x_{16} = \langle \underline{0256} \rangle, \langle 1347 \rangle$
$x_{17} = \langle \underline{0257} \rangle, \langle 0267 \rangle, \langle 1247 \rangle, \langle 2347 \rangle$
$x_{18} = \langle \underline{0567} \rangle, \langle 1234 \rangle$
$x_{19} = \langle 1237 \rangle, \langle 2567 \rangle$
$x_{20} = \langle 1256 \rangle, \langle 1357 \rangle, \langle 1367 \rangle, \langle 2356 \rangle$
$x_{21} = \langle 1257 \rangle, \langle 2367 \rangle$
$x_{22} = \langle 1267 \rangle, \langle 2357 \rangle$
$x_{23} = \langle 1356 \rangle$
$x_{24} = \langle \underline{012345} \rangle, \langle 012346 \rangle, \langle \underline{014567} \rangle, \langle 034567 \rangle$
$x_{25} = \langle \underline{012347} \rangle, \langle \underline{024567} \rangle$
$x_{26} = \langle \underline{012356} \rangle, \langle 134567 \rangle$
$x_{27} = \langle \underline{012357} \rangle, \langle 012367 \rangle, \langle 124567 \rangle, \langle 234567 \rangle$
$x_{28} = \langle \underline{012456} \rangle, \langle \underline{013457} \rangle, \langle 013467 \rangle, \langle 023456 \rangle$
$x_{29} = \langle \underline{012457} \rangle, \langle 023467 \rangle$
$x_{30} = \langle \underline{012467} \rangle, \langle 023457 \rangle$
$x_{31} = \langle \underline{012567} \rangle, \langle 023567 \rangle, \langle 123457 \rangle, \langle 123467 \rangle$
$x_{32} = \langle \underline{013456} \rangle$
$x_{33} = \langle \underline{013567} \rangle, \langle 123456 \rangle$
$x_{34} = \langle 123567 \rangle$
$x_{35} = \langle \underline{01234567} \rangle$

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and 5 are common to the previous cluster, and only sites enumerated as 8 and 9 are newly considered. The motivations for choosing this cluster are its spatial compactness and, due to its overlapping the former cluster, many correlations are already known, thereby hopefully sufficient to determine more easily many new solutions. Following the same procedure as mentioned, it is observed that 38 nonequivalent multispin correlations exhaust all possibilities (see Table II). Of these, thirteen correlations are known (from previous cluster calculation). Twenty-six possible identities are developed for this cluster and are the following:

$$A(w_1 + w_2) + B(w_{11} + w_{12} + w_{13} + w_{14}) = x_4 - A(x_2 + x_3), \quad (3.35)$$

$$A(w_3 + w_4) + B(w_5 + w_6 + w_{10} + w_{22}) = x_7 - A(x_1 + x_6), \quad (3.36)$$

$$2Aw_7 + 2B(w_{16} + w_{19}) = x_8 - 2Ax_6, \quad (3.37)$$

$$A(w_5 + w_6) + B(w_3 + w_4 + w_{10} + w_{22}) = x_{10} - A(x_1 + x_6), \quad (3.38)$$

$$A(w_{13} + w_{14}) + B(w_1 + w_2 + w_{11} + w_{12}) = x_{13} - A(x_2 + x_3), \quad (3.39)$$

$$A(w_{11} + w_{12}) + B(w_{11} + w_{12} + w_{15} + w_{24}) = x_{14} - A(x_2 + x_{18}), \quad (3.40)$$

$$-w_3 + A(w_1 + w_{11} + w_{13}) + B(w_2 + w_{12} + w_{14}) = -Ax_2 - Bx_3, \quad (3.41)$$

$$-w_4 + A(w_2 + w_{12} + w_{14}) + B(w_1 + w_{11} + w_{13}) = -Ax_3 - Bx_2, \quad (3.42)$$

$$-w_5 + A(w_2 + w_{11} + w_{14}) + B(w_1 + w_{12} + w_{13}) = -Ax_2 - Bx_3, \quad (3.43)$$

TABLE II. Definitions of spin correlations upon the eight-site cluster shown in Fig. 2(b) where the underlined correlations are used as generators for correlation identities.

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$x_1 = \langle 01 \rangle, \langle 02 \rangle, \langle 03 \rangle, \langle 04 \rangle, \langle 15 \rangle, \langle 45 \rangle, \langle 58 \rangle, \langle 59 \rangle$
$x_2 = \langle 05 \rangle, \langle 12 \rangle, \langle 14 \rangle, \langle 18 \rangle, \langle 23 \rangle, \langle 34 \rangle, \langle 49 \rangle, \langle 89 \rangle$
$x_3 = \langle 13 \rangle, \langle 19 \rangle, \langle 24 \rangle, \langle 48 \rangle$
$x_4 = \langle \underline{08} \rangle, \langle 09 \rangle, \langle 25 \rangle, \langle 35 \rangle$
$w_1 = \langle 28 \rangle, \langle 39 \rangle$
$w_2 = \langle 29 \rangle, \langle 38 \rangle$
$x_6 = \langle 0123 \rangle, \langle 0124 \rangle, \langle 0134 \rangle, \langle 0234 \rangle, \langle 1458 \rangle, \langle 1459 \rangle, \langle 1589 \rangle, \langle 4589 \rangle$
$x_7 = \langle 0125 \rangle, \langle \underline{0158} \rangle, \langle 0345 \rangle, \langle 0459 \rangle$
$x_8 = \langle 0235 \rangle, \langle \underline{0589} \rangle$
$x_{10} = \langle 0135 \rangle, \langle \underline{0159} \rangle, \langle 0245 \rangle, \langle 0458 \rangle$
$x_{12} = \langle 0145 \rangle$
$x_{13} = \langle \underline{0148} \rangle, \langle 0149 \rangle, \langle 1245 \rangle, \langle 1345 \rangle$
$x_{14} = \langle \underline{0189} \rangle, \langle 0489 \rangle, \langle 1235 \rangle, \langle 2345 \rangle$
$x_{18} = \langle 1234 \rangle, \langle 1489 \rangle$
$w_3 = \langle \underline{0128} \rangle, \langle 0349 \rangle, \langle 1258 \rangle, \langle 3459 \rangle$
$w_4 = \langle \underline{0129} \rangle, \langle 0348 \rangle, \langle 1358 \rangle, \langle 2459 \rangle$
$w_5 = \langle \underline{0138} \rangle, \langle 0249 \rangle, \langle 1259 \rangle, \langle 3458 \rangle$
$w_6 = \langle \underline{0139} \rangle, \langle 0248 \rangle, \langle 1359 \rangle, \langle 2458 \rangle$
$w_7 = \langle \underline{0238} \rangle, \langle 0239 \rangle, \langle 2589 \rangle, \langle 3589 \rangle$
$w_8 = \langle \underline{0258} \rangle, \langle 0359 \rangle$
$w_9 = \langle \underline{0259} \rangle, \langle 0358 \rangle$
$w_{10} = \langle \underline{0289} \rangle, \langle 0389 \rangle, \langle 2358 \rangle, \langle 2359 \rangle$
$w_{11} = \langle 1238 \rangle, \langle 1289 \rangle, \langle 2349 \rangle, \langle 3489 \rangle$
$w_{12} = \langle 1239 \rangle, \langle 1389 \rangle, \langle 2348 \rangle, \langle 2489 \rangle$
$w_{13} = \langle 1248 \rangle, \langle 1349 \rangle$
$w_{14} = \langle 1249 \rangle, \langle 1348 \rangle$
$w_{15} = \langle 2389 \rangle$
$x_{24} = \langle 012345 \rangle, \langle \underline{014589} \rangle$
$w_{16} = \langle \underline{012348} \rangle, \langle 012349 \rangle, \langle 124589 \rangle, \langle 134589 \rangle$
$w_{17} = \langle \underline{012358} \rangle, \langle \underline{012589} \rangle, \langle 023459 \rangle, \langle 034589 \rangle$
$w_{18} = \langle \underline{012359} \rangle, \langle \underline{013589} \rangle, \langle 023458 \rangle, \langle 024589 \rangle$
$w_{19} = \langle \underline{012389} \rangle, \langle 023489 \rangle, \langle 123589 \rangle, \langle 234589 \rangle$
$w_{20} = \langle \underline{012458} \rangle, \langle 013459 \rangle$
$w_{21} = \langle \underline{012459} \rangle, \langle 013458 \rangle$
$w_{22} = \langle \underline{012489} \rangle, \langle 013489 \rangle, \langle 123458 \rangle, \langle 123459 \rangle$
$w_{23} = \langle \underline{023589} \rangle$
$w_{24} = \langle 123489 \rangle$
$w_{25} = \langle \underline{01234589} \rangle$

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$$-w_6 + A(w_1 + w_{12} + w_{13}) + B(w_2 + w_{11} + w_{14}) = -Ax_3 - Bx_2, \quad (3.44)$$

$$-w_7 + A(w_1 + w_2 + w_{11} + w_{12}) + B(w_{13} + w_{14}) = -B(x_2 + x_3), \quad (3.45)$$

$$-w_8 + A(w_3 + w_6 + w_{10}) + B(w_4 + w_5 + w_{22}) = -Ax_1 - Bx_6, \quad (3.46)$$

$$-w_9 + A(w_4 + w_5 + w_{10}) + B(w_3 + w_6 + w_{22}) = -Ax_1 - Bx_6, \quad (3.47)$$

$$-w_{10} + A(w_{11} + w_{12} + w_{15}) + B(w_{11} + w_{12} + w_{24}) = -Ax_2 - Bx_{18}, \quad (3.48)$$

$$2Aw_{16} + 2B(w_7 + w_{19}) = x_{24} - 2Ax_6, \quad (3.49)$$

$$-w_{16} + A(w_{11} + w_{12} + w_{13} + w_{14}) + B(w_1 + w_2) = -B(x_2 + x_3), \quad (3.50)$$

$$-w_{17} + A(w_3 + w_4 + w_{10} + w_{22}) + B(w_5 + w_6) = -B(x_1 + x_6), \quad (3.51)$$

$$-w_{17} + (A+B)(w_7 + w_{16} + w_{19}) = -(A+B)x_6, \quad (3.52)$$

$$-w_{18} + A(w_5 + w_6 + w_{10} + w_{22}) + B(w_3 + w_4) = -B(x_1 + x_6), \quad (3.53)$$

$$-w_{18} + (A+B)(w_7 + w_{16} + w_{19}) = -(A+B)x_6, \quad (3.54)$$

$$-w_{19} + A(w_{11} + w_{12} + w_{15} + w_{24}) + B(w_{11} + w_{12}) = -B(x_2 + x_{18}), \quad (3.55)$$

$$-w_{20} + A(w_3 + w_6 + w_{22}) + B(w_4 + w_5 + w_{10}) = -Ax_6 - Bx_1, \quad (3.56)$$

$$-w_{21} + A(w_4 + w_5 + w_{22}) + B(w_3 + w_6 + w_{10}) = -Ax_6 - Bx_1, \quad (3.57)$$

$$-w_{22} + A(w_{11} + w_{12} + w_{24}) + B(w_{11} + w_{12} + w_{15}) = -Ax_{18} - Bx_2, \quad (3.58)$$

$$-w_{23} + 2A(w_7 + w_{19}) + 2Bw_{16} = -2Bx_6, \quad (3.59)$$

$$-w_{25} + 2A(w_{16} + w_{19}) + 2Bw_7 = -2Bx_6. \quad (3.60)$$

Investigation shows again, that to obtain a nonvanishing determinant of the coefficient matrix, one needs knowledge of six correlation solutions (in addition to the already known 13 correlations). These are taken to be  $w_3, w_4, w_5, w_6, w_{10}$ , and  $w_{14}$ , where all are four-spin correlations. The latter six correlations are presently calculated by Pfaffian techniques thus enabling the system of linear-algebraic equations to be solved exactly for the remaining 19 unknown correlations.

As results, the graphs of pair correlations (five shortest distances) versus reduced temperature  $T/T_c$  are shown in Fig. 3. Beginning at unity saturation values, all correla-

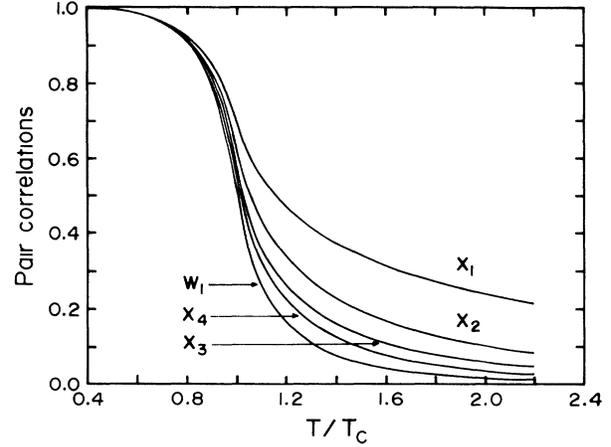


FIG. 3. Exact solutions for pair correlations of the square Ising model as functions of the reduced temperature  $K_c/K (= T/T_c)$ , where  $K_c = \frac{1}{2} \ln(\sqrt{2} + 1) = 0.44068\dots$ , and where, in order of increasing radial distance  $x_1 = \langle 01 \rangle$ ,  $x_2 = \langle 05 \rangle$ ,  $x_3 = \langle 07 \rangle$ ,  $x_4 = \langle 16 \rangle$ , and  $w_1 = \langle 28 \rangle$ .

tions are continuous monotonically decreasing functions of temperature tending to zero at high temperatures. At the critical temperature  $T = T_c$ , there is in each case a vertical inflection point as a weak singularity of energy type  $\epsilon \ln \epsilon$ , where  $\epsilon \equiv |T - T_c|/T_c$ . As expected, the curve for the nearest-neighbor pair correlation  $x_1$  (energy) forms an upper envelope for all even-number correlation curves.

In addition, the seven shortest-distance pair correlations are plotted in Fig. 4 as functions of radial distance at three different temperatures  $T/T_c = 0.9580, 1.0000$ , and  $1.1017$ , where these graphs reveal monotonically decreasing behavior versus radial distance, which agree and extend upon the results of Kaufman and Onsager<sup>8</sup> who plotted the five shortest distance pair correlations as functions of radial distance.

Next, four multispin correlations are plotted as functions of reduced temperature. These are select pair-, quartet-, sextet-, and octet-correlations (see Fig. 5). As

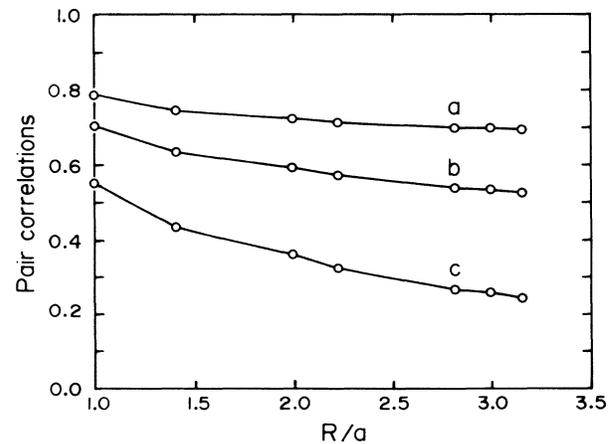


FIG. 4. Exact solutions for the pair correlation of the square Ising model as functions of relative radial distance  $R/a$  ( $a$  being lattice spacing) at three different temperatures: curve  $a$ ,  $T/T_c = 0.9580$ ; curve  $b$ ,  $T/T_c = 1.0000$ ; curve  $c$ ,  $T/T_c = 1.1017$ .

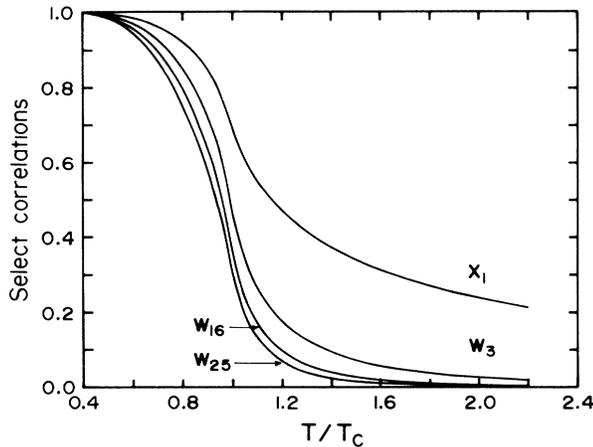


FIG. 5. Exact solutions for select even-number correlations of the square Ising model as functions of the reduced temperature  $T/T_c$ , where  $x_1 = \langle 01 \rangle$ ,  $w_3 = \langle 0128 \rangle$ ,  $w_{16} = \langle 012348 \rangle$ , and  $w_{25} = \langle 01234589 \rangle$ .

expected, all correlations are continuous monotonically decreasing functions of temperature and have the same types of qualitative behavior as the nearest-neighbor pair correlation.

The exact solutions for the correlations defined upon each of the eight-site clusters previously shown in Fig. 2 offer two examples of essential-type degeneracies. From the systems of linear-algebraic equations, one can immediately establish by inspection [see Eqs. (3.7), (3.10), (3.52), and (3.54)] that

$$x_7 = x_{10}, \quad w_{17} = w_{18}, \quad (3.61)$$

where the former (latter) is between quartet (sextet) correlations. As is easily seen in Fig. 6, these essentially degenerate correlations are geometrically inequivalent, but, in fact, their values are identical for all temperatures (or

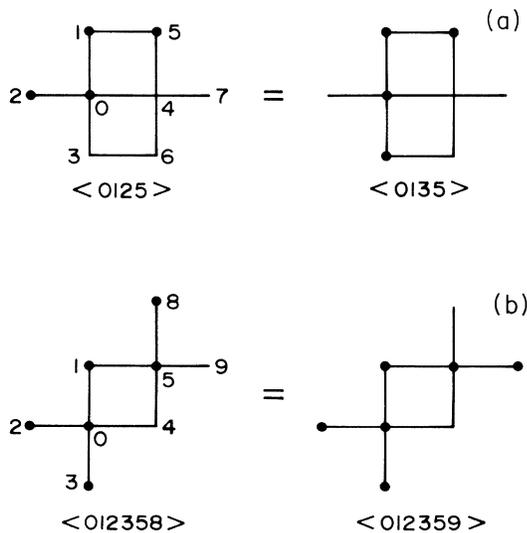


FIG. 6. Diagrammatic illustrations of essential-type degeneracies, specifically, twofold degeneracies between (a) quartet and (b) sextet correlations.

for all values of dimensionless interaction parameter). Moreover, superimposing Figs. 3 and 5 reveals an accidental-type (crossing point) degeneracy between the correlations  $w_1$  and  $w_3$ . A complete statistical-mechanical theory of degeneracies for multispin correlations does not yet exist.

The present method and its success for determining large numbers of exact solutions for Ising correlations offer some insights for further advances along similar directions. For example, in the calculational systematics, choosing a spatially compact cluster of sites whose associated correlations appreciably overlap presently known correlations would appear to be a desirable strategy since one then needs to handle fewer unknowns, thus raising more favorable expectations concerning closure and linear-independent requirements.

#### IV. SUMMARY AND CONCLUSIONS

The present theoretical investigations have developed and demonstrated a method for obtaining large numbers of exact solutions for  $n$ -site ( $n$ -even-integer) localized Ising correlations on the square lattice. Combining usual Pfaffian techniques with linear-algebraic systems of correlation identities, the method is reasonably straightforward with computer aid and indeed much simpler and more fruitful than using Pfaffian procedures exclusively. Some of the successes are evidenced by the facts that *sixty* (exhaustive in number upon each of two eight-site clusters) exact solutions were determined and the eight-site correlation solutions are, to our knowledge the first of that order to be explicitly evaluated for an Ising model on any regular planar lattice. In addition, since the square lattice is "loose-packed," it should be mentioned that exact correlation solutions for the square Ising *antiferromagnet* can now be obtained by merely inverting the appropriate ferromagnetic solutions.

Upon examining a typical system of linear identities involving all correlations defined upon a given cluster of sites, one most often finds that linear independence is a more elusive algebraic property than closure. Consequently, one secures a linearly independent subset of equations by searching for and then calculating a selection of the unknown correlations by Pfaffian methods thereby reducing the number of unknowns in the original system. Any resulting subset (or subsets) of linearly independent equations can then be solved by standard linear algebraic and related numerical procedures. Significantly, the entire search and numerical analyses were made highly efficient and benefited from an original Fortran program designed to find and triangularize an appropriate coefficient matrix which circumvented enormously large combinatorics and entailed very short computer time.

Generally, if a very large sample set is assembled for scientific observation, one may hope to uncover some special features not discernible within a small sample set. However, for the case of even-number correlations of planar Ising models, it has been difficult in practice to obtain large numbers of exact solutions since conventional Pfaffian techniques involving rather complicated expres-

sions of elliptic integrals and Toeplitz determinants become progressively lengthy and very laborious as either the numbers of sites under consideration or the distance between these sites increase. The methods of the present paper have succeeded to a sizable extent in traversing this calculational impasse enabling new correlation information to be explored for the square Ising model in zero magnetic field ("Onsager lattice"). As illustrations, besides the anticipated behaviors that Ising model even-number correlations are continuous monotonically decreasing functions of temperature exhibiting weak (energy-type) singularities at the critical temperature, examples of both essential- and accidental-type degeneracies are exposed upon examining many exact correlation solutions. Although these occurrences of degeneracies have strictly only been established here for the square Ising magnet, one can likely infer similar incidents for other lattice structures.

Allying the types of procedures in the present paper with extended transformation theorems (extended in the

sense that the theorems are applied beyond partition functions to multisite correlations), exact solutions have also been obtained for Ising-model correlations on other planar lattices<sup>18</sup> (regular and irregular) and these results along with some examples of applications have been published.<sup>19</sup> Notably, therefore, the present and previous results<sup>18</sup> now enable exact solutions to be obtained in an efficient and systematic manner for Ising localized even-number correlations upon *all* two-dimensional regular lattices (honeycomb, square, kagomé, and triangular) as well as upon their bond-decorated (irregular) lattices. With such availability of exact solutions for localized Ising correlations (magnet, lattice gas, binary alloy, etc.) on various planar lattices, there are, in fact, some interesting and informative thermal quantities, both in equilibrium and nonequilibrium, which are largely local in their character and which can now be more thoroughly investigated and compared upon different planar lattice structures with perhaps some special and diverse effects of their own to reveal.

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<sup>1</sup>G. E. Newell and E. W. Montroll, *Rev. Mod. Phys.* **25**, 353 (1953); S. G. Brush, *ibid.* **39**, 883 (1967); H. N. V. Temperley, in *Phase Transition and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 1; B. M. McCoy and T. T. Wu, *The Two-Dimensional Ising Model* (Harvard University Press, Cambridge, Mass., 1973); M. E. Fisher, *Physica A* **106**, 28 (1981).

<sup>2</sup>W. L. Bragg and E. J. Williams, *Proc. R. Soc. (London) Ser. A* **145**, 699 (1934).

<sup>3</sup>C. N. Yang and T. D. Lee, *Phys. Rev.* **87**, 404 (1952); **87**, 410 (1952).

<sup>4</sup>C. J. Thompson, *Mathematical Statistical Mechanics* (Macmillan, New York, 1972).

<sup>5</sup>H. A. Kramers and G. H. Wannier, *Phys. Rev.* **60**, 252 (1941).

<sup>6</sup>E. W. Montroll, *J. Chem. Phys.* **9**, 706 (1941).

<sup>7</sup>L. Onsager, *Phys. Rev.* **65**, 117 (1944).

<sup>8</sup>B. Kaufman and L. Onsager, *Phys. Rev.* **76**, 1244 (1949).

<sup>9</sup>C. N. Yang, *Phys. Rev.* **85**, 808 (1952).

<sup>10</sup>C. H. Munera, Ph.D. thesis, Ohio University, 1982 (unpublished).

<sup>11</sup>(a) G. D. Mahan, *Phys. Rev. B* **14**, 780 (1976); (b) N. L. Sharma and T. Tanaka, *ibid.* **28**, 2146 (1983); (c) T. Tanaka, M. A. Sawtarie, J. H. Barry, N. L. Sharma, and C. H. Munera, *ibid.* **34**, 3773 (1986).

<sup>12</sup>M. Thomsen, M. F. Thorpe, T. C. Choy, and D. Sherrington, *Phys. Rev. B* **30**, 250 (1984).

<sup>13</sup>C. A. Hurst and H. S. Green, *J. Chem. Phys.* **33**, 1059 (1960); W. Kasteleyn, *J. Math.* **4**, 287 (1963); E. W. Montroll, in *Applied Combinatorial Mathematics*, edited by E. F. Bechkenbach (Wiley, New York, 1964); E. W. Montroll, R. B. Potts, and J. C. Ward, *J. Math. Phys.* **4**, 308 (1963); H. S. Green and C. A. Hurst, *Order-Disorder Phenomena* (Wiley, New York,

1964); J. Stephenson, *J. Math. Phys.* **5**, 1009 (1964); **7**, 1123 (1966); P. W. Kasteleyn, in *Graph Theory and Theoretical Physics*, edited by F. Harary (Academic, London, 1967); B. McCoy and T. T. Wu, *The Two-Dimensional Ising Model*, Ref. 1.

<sup>14</sup>B. M. McCoy, C. A. Tracy, and T. T. Wu, *Phys. Rev. Lett.* **38**, 793 (1977).

<sup>15</sup>H. Au-Yang and J. H. Perk, *Phys. Lett.* **104A**, 131 (1984).

The exact solutions for the pair correlations  $x_1, x_2, x_3, x_4, x_5, w_1$ , and  $w_2$  in the present paper have also been checked against their critical values given in this reference: R. K. Ghosh and R. E. Shrock, *Phys. Rev. B* **30**, 3790 (1984); *J. Stat. Phys.* **38**, 473 (1985); *Phys. Rev. B* **31**, 1486 (1985); K. Yamada, *Prog. Theor. Phys.* **71**, 1416 (1984); **72**, 922 (1984); **76**, 602 (1986); **76**, 613 (1986).

<sup>16</sup>M. E. Fisher, *Phys. Rev.* **113**, 696 (1959); H. B. Callen, *Phys. Lett.* **4**, 161 (1963); M. Suzuki, *ibid.* **19**, 267 (1965); C. Gruber and D. Merlini, *Physica* **67**, 308 (1973); J. H. Barry, C. H. Munera, and T. Tanaka, *Physica A* **113**, 367 (1982). Some errors in the last reference have been pointed out by T. C. Choy.

<sup>17</sup>J. S. Vandergraft, *Introduction to Numerical Computations* (Academic, New York, 1978). In the present study, a new FORTRAN program has been developed to treat rectangular coefficient matrices with aid of this reference

<sup>18</sup>J. H. Barry, M. Khatun, and T. Tanaka, *Phys. Rev. B* **37**, 5193 (1988); M. Khatun, Ph.D. thesis, Ohio University, 1985 (unpublished); *Bull. Am. Phys. Soc.* **30**, 596 (1985).

<sup>19</sup>To illustrate, using localized correlation solutions, the initial perpendicular susceptibilities of the kagomé and decorated-kagomé Ising models have been exactly calculated: J. H. Barry and M. Khatun, *Phys. Rev. B* **35**, 8601 (1987). Application of localized honeycomb Ising correlations to the superionic conductivity of the solid electrolyte  $\text{AgCrS}_2$  can be found in Refs. 11(b) and 11(c).