Exact solutions for perpendicular susceptibilities of kagomé and decorated-kagomé Ising models

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For more than two decades, exact and explicit solutions for the initial isothermal transverse susceptibility $\chi_\perp(T)$ of the quantum-mechanical Ising model ferromagnet have been known on the honeycomb, square, and triangular lattices but not as yet on the kagomé lattice which is the only other regular lattice in two dimensions. Recently, however, exact solutions have been found for localized even-number correlations of the ferromagnetic kagomé Ising model, rendering its $\chi_\perp(T)$ exactly calculable. Similar to the other three regular lattices, the resulting continuous curve for $\chi_\perp(T)/\chi_\perp(0)$ shows both a weak (energy-type) singularity at the critical temperature T_c where $\chi_\perp(T_c)/\chi_\perp(0)=1.1426\ldots$ and a rounded maximum at $T_{\max}>T_c$ with the parameters of this maximum given by $\chi_\perp^{\max}/\chi_\perp(0)=1.1945\ldots$ at $T_{\max}/T_c=1.0994\ldots$. The exact solution for $\chi_\perp(T)$ of the decorated-kagomé Ising-model ferromagnet is also obtained having modified features illustrating the effects of the decoration spins (singly decorated bonds) upon $\chi_\perp(T)$.

I. INTRODUCTION

Investigating planar Ising models on regular lattices in the presence of a transverse magnetic field, Fisher[1] used graph-theoretical arguments to establish an exact closed formula for the initial isothermal transverse susceptibility $\chi_\perp(T)$ and proceeded, in particular, to demonstrate its explicit solutions on the two-dimensional honeycomb and square lattice structures. After first calculating the necessary Ising correlations by Pfaffian techniques, Stephenson[2] then applied the same formula to find the exact solution for $\chi_\perp(T)$ on the triangular lattice. Pursuing a different (non-graph-theoretic) approach, Horiguchi and Morita[3] generalized the formula to include both regular and irregular lattices of arbitrary spatial dimensionality and applied their generalized formula to obtain $\chi_\perp(T)$ exactly on a regular Cayley tree. The present theoretical investigations combine essential features of the analytical method of Horiguchi and Morita with recently developed methods[4] for securing exact solutions of Ising multisite correlations on planar lattices, thereby enabling $\chi_\perp(T)$ to be determined exactly upon both the kagomé and decorated-kagomé lattice structures.

The traditional Ising-model ferromagnet is defined upon a lattice of N sites as the Hamiltonian

$$\mathcal{H}_0=-J\sum_{\langle i,j\rangle}\sigma_i\sigma_j \ , \tag{1.1}$$

where each site-localized Ising variable $\sigma_l=\pm1$, $\sum_{\langle i,j\rangle}\cdots$ designates summation over all distinct nearest-neighbor pairs of lattice sites and $J>0$ is the strength parameter of the ferromagnetic interaction. Viewing the σ_i variables as z-component Pauli spin operators, the model becomes quantum-mechanical in the presence of a transverse magnetic field since the Hamiltonian then contains noncommuting operators. For more than two decades,[1,2] exact and explicit solutions for the initial isothermal transverse susceptibility $\chi_\perp(T)$ of the quantum-mechanical Ising model have been known on the honeycomb, square, and triangular lattices but not as yet on the kagomé lattice which is the only other regular (all sites equivalent, all bonds equivalent) lattice in two dimensions. As previously mentioned, however, exact solutions have recently[4] been obtained for localized even-number correlations of the ferromagnetic kagomé Ising model rendering its $\chi_\perp(T)$ exactly calculable. Also, aided by newly[4] developed extended transformation theorems and results which map Ising correlations of irregular (bond-decorated) lattices upon linear combinations of Ising correlations belonging to the original regular lattices, the exact solution for $\chi_\perp(T)$ of the decorated-kagomé Ising model ferromagnet is then obtained having modified features illustrating the effects of the bond-decoration spins upon $\chi_\perp(T)$.

II. EXACT FORMULA FOR $\chi_\perp(T)$ OF THE ISING MODEL ON REGULAR AND IRREGULAR LATTICES

In the present section, some essential aspects of the analytical method of Horiguchi and Morita[3] will be adopted to develop in a self-contained manner an exact and convenient representation for $\chi_\perp(T)$ on regular or irregular lattices of arbitrary spatial dimensionality.

Consider the system Hamiltonian

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1 \ , \tag{2.1}$$

where

$$\mathcal{H}_0=-J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z \tag{2.2}$$

is the standard Ising model (1.1) introduced earlier whose variables are now represented by z-component Pauli spin operators, and

$$\mathcal{H}_1 = -h_x \sum_i \sigma_i^x = -h_x M_x \tag{2.3}$$

represents the interaction energy[5] of the spin system with the transverse uniform, static, external magnetic field h_x, where σ_i^x is the x-component Pauli spin operator localized on the ith lattice site and $M_x = \sum_i \sigma_i^x$ is the x-component magnetic moment operator of the system. Letting the set of all z-component Pauli spin operators $\{\sigma_0^z, \sigma_1^z, \ldots, \sigma_{N-1}^z\} \equiv \sigma$, the magnetic canonical partition function Z is given by the usual trace formula over all degrees of freedom of the system

$$Z = \operatorname*{Tr}_{\sigma} e^{-\beta\mathcal{H}} \tag{2.4}$$

whose inverse appears as the normalization factor in the expression for the canonical thermal average

$$\langle M_x \rangle_{h_x} = Z^{-1} \operatorname*{Tr}_{\sigma} M_x e^{-\beta\mathcal{H}} , \tag{2.5}$$

where $\beta = 1/k_B T$ with k_B being the Boltzmann constant, T the absolute temperature, and where the subscript h_x on the thermal average symbol emphasizes that the thermal averaging is performed using a Hamiltonian containing a finite magnetic field $h_x > 0$. In contrast, a thermal average symbol devoid of any such subscript will signify that the thermal averaging is performed in the absence of a transverse magnetic field ($h_x = 0$). The *initial isothermal transverse susceptibility* $\chi_\perp(T)$ is now defined by

$$\chi_\perp(T) = \lim_{h_x \to 0} \frac{\partial \langle M_x \rangle_{h_x}}{\partial h_x} . \tag{2.6}$$

In order to derive an exact and useful formula for $\chi_\perp(T)$, one first presents the following standard theorem where A,B are operators together with its short proof.

Theorem:

$$e^{-\beta(A+B)} = e^{-\beta A} - \int_0^\beta d\lambda\, e^{-(\beta-\lambda)A} B e^{-\lambda(A+B)} . \tag{2.7}$$

Proof: Let $f(\beta) \equiv e^{\beta A} e^{-\beta(A+B)}$. Then differentiating gives

$$\begin{aligned} f'(\beta) &= e^{\beta A} A e^{-\beta(A+B)} - e^{\beta A}(A+B) e^{-\beta(A+B)} \\ &= -e^{\beta A} B e^{-\beta(A+B)} . \end{aligned}$$

By integrating both sides from 0 to β and then multiplying by $e^{-\beta A}$, one obtains (2.7) completing the proof of the theorem.

The above theorem is actually an integral equation representation for $e^{-\beta(A+B)}$, where most commonly A,B are noncommuting operators, and, as such, is a familiar form for initiating perturbation theory in quantum statistical mechanics.[6] In this context, the type of integral equation (2.7) (linear, inhomogeneous, Volterra, second kind) can be formally solved by the method of successive iterations which gives

$$e^{-\beta(A+B)} = e^{-\beta A} - \int_0^\beta d\lambda\, e^{-(\beta-\lambda)A} B e^{-\lambda A} + \cdots \tag{2.8}$$

enabling one to derive an exact formula for $\chi_\perp(T)$ of Ising models on both regular and irregular lattices of arbitrary spatial dimensionality as now will be shown.

Defining

$$Z_0 = \operatorname*{Tr}_{\sigma} e^{-\beta\mathcal{H}_0} \tag{2.9}$$

and using (2.1)–(2.5) and (2.8), one obtains

$$\begin{aligned} \langle M_x \rangle_{h_x} &= Z^{-1} \operatorname*{Tr}_{\sigma} M_x e^{-\beta\mathcal{H}} = \frac{\operatorname*{Tr}_{\sigma} M_x e^{-\beta(\mathcal{H}_0+\mathcal{H}_1)}}{\operatorname*{Tr}_{\sigma} e^{-\beta(\mathcal{H}_0+\mathcal{H}_1)}} \\ &= \frac{\operatorname*{Tr}_{\sigma} M_x \left[e^{-\beta\mathcal{H}_0} - \int_0^\beta d\lambda\, e^{-(\beta-\lambda)\mathcal{H}_0} \mathcal{H}_1 e^{-\lambda\mathcal{H}_0} + \cdots \right]}{\operatorname*{Tr}_{\sigma} \left[e^{-\beta\mathcal{H}_0} - \int_0^\beta d\lambda\, e^{-(\beta-\lambda)\mathcal{H}_0} \mathcal{H}_1 e^{-\lambda\mathcal{H}_0} + \cdots \right]} \\ &= \frac{\operatorname*{Tr}_{\sigma} M_x e^{-\beta\mathcal{H}_0} - \operatorname*{Tr}_{\sigma} M_x \int_0^\beta d\lambda\, e^{-(\beta-\lambda)\mathcal{H}_0} \mathcal{H}_1 e^{-\lambda\mathcal{H}_0} + O(h_x^3)}{Z_0 + O(h_x^2)} \\ &= -Z_0^{-1} \int_0^\beta d\lambda \operatorname*{Tr}_{\sigma} (e^{\lambda\mathcal{H}_0} \mathcal{H}_1 e^{-\lambda\mathcal{H}_0} M_x e^{-\beta\mathcal{H}_0}) + O(h_x^3) , \end{aligned} \tag{2.10}$$

where, in writing the last expression (2.10), one has used the fact that

$$\langle M_x \rangle = Z_0^{-1} \operatorname*{Tr}_{\sigma} M_x e^{-\beta\mathcal{H}_0} = 0 ,$$

as well as the invariance property of a trace under cyclic permutations, and has chosen to interchange the order of the λ-integration and thermal-averaging procedures. Substituting (2.3) into (2.10) one obtains

$$\langle M_x \rangle_{h_x} = h_x \int_0^\beta d\lambda \langle M_x(-i\lambda) M_x \rangle + O(h_x^3) , \tag{2.11}$$

where

$$A(-i\lambda)\equiv e^{\lambda\mathcal{H}_0}Ae^{-\lambda\mathcal{H}_0}$$

is the definition of an operator A in the "temperature-interaction representation." Recalling the definition (2.6) for $\chi_\perp(T)$, (2.11) then directly yields

$$\chi_\perp(T)=\int_0^\beta d\lambda\langle M_x(-i\lambda)M_x\rangle=\sum_{r,s}\int_0^\beta d\lambda\langle\sigma_r^x(-i\lambda)\sigma_s^x\rangle \tag{2.12}$$

having written $M_x=\sum_r \sigma_r^x$ for the x-component magnetic moment operator of the system. Following Horiguchi and Morita,[3] the expression (2.12) can be further simplified using the two identities:

$$f(\{\sigma_n^z\})\sigma_k^x=\sigma_k^x f(\{(-1)^{\delta_{nk}}\sigma_n^z\})\ , \tag{2.13a}$$

$$\operatorname*{Tr}_\sigma \sigma_l^x\sigma_k^x f(\{\sigma_n^z\})=\delta_{lk}\operatorname*{Tr}_\sigma f(\{\sigma_n^z\})\ , \tag{2.13b}$$

where δ_{pq} is the usual Kronecker delta symbol and $f(\{\sigma_n^z\})$ is any function of the σ_i^z operators. The proofs of both identities (2.13) are actually quite straightforward, namely, (2.13a) is proven by using elementary properties of the Pauli spin algebra and (2.13b) by conveniently choosing a product representation in which all σ_i^z operators of the system are diagonal. Proceeding, therefore, to use (2.13a) and (2.13b), the thermal average in (2.12) becomes

$$\begin{aligned}\langle\sigma_r^x(-i\lambda)\sigma_s^x\rangle&=\langle e^{\lambda\mathcal{H}_0}\sigma_r^x e^{-\lambda\mathcal{H}_0}\sigma_s^x\rangle\\&=Z_0^{-1}\operatorname*{Tr}_\sigma e^{\lambda\mathcal{H}_0}\sigma_r^x e^{-\lambda\mathcal{H}_0}\sigma_s^x e^{-\beta\mathcal{H}_0}\\&=Z_0^{-1}\delta_{rs}\operatorname*{Tr}_\sigma e^{-2\lambda J\sigma_s^z\sum_1^q\sigma_{s'}^z}e^{-\beta\mathcal{H}_0}\\&=\delta_{rs}\langle e^{-2\lambda J\sigma_s^z\sum_1^q\sigma_{s'}^z}\rangle\ ,\end{aligned} \tag{2.14}$$

where use has also been made of the definition (2.2) for the Ising Hamiltonian $\mathcal{H}_0$ as well as the corresponding canonical thermal average. In (2.14), the summation sites s' are the nearest-neighbor sites of site s, and q is the number of nearest-neighboring sites of s [one remarks that q need not be a constant, e.g., $q=q(s)$ for an irregular lattice having nonequivalent sites]. Substituting (2.14) into (2.12) gives

$$\begin{aligned}\chi_\perp(T)&=\sum_{r,s}\int_0^\beta d\lambda\langle\sigma_r^x(-i\lambda)\sigma_s^x\rangle\\&=\sum_r\int_0^\beta d\lambda\langle e^{-2\lambda J\sigma_r^z\sum_1^q\sigma_{r'}^z}\rangle\ ,\end{aligned}$$

whereupon now electing to first perform the λ integration (contrasting the choice of Horiguchi and Morita) yields

$$\chi_\perp(T)=\sum_r\left\langle\frac{1-e^{-2\beta J\sigma_r^z\sum_1^q\sigma_{r'}^z}}{2J\sigma_r^z\sum_1^q\sigma_{r'}^z}\right\rangle\ . \tag{2.15}$$

Letting $\mathcal{H}_0',\mathrm{Tr}_\sigma'$ denote a *restricted* Hamiltonian and trace operation, respectively, which *exclude* site r, one next rewrites the summand of (2.15) as

$$\begin{aligned}\left\langle\frac{1-e^{-2\beta J\sigma_r^z\sum_1^q\sigma_{r'}^z}}{2J\sigma_r^z\sum_1^q\sigma_{r'}^z}\right\rangle&=Z_0^{-1}\operatorname*{Tr}_\sigma\exp(-\beta\mathcal{H}_0)\frac{1-e^{-2\beta J\sigma_r^z\sum_1^q\sigma_{r'}^z}}{2J\sigma_r^z\sum_1^q\sigma_{r'}^z}=Z_0^{-1}\operatorname*{Tr}_\sigma\exp(-\beta\mathcal{H}_0')\frac{e^{\beta J\sigma_r^z\sum_1^q\sigma_{r'}^z}-e^{-\beta J\sigma_r^z\sum_1^q\sigma_{r'}^z}}{2J\sigma_r^z\sum_1^q\sigma_{r'}^z}\\&=Z_0^{-1}\operatorname*{Tr'}_\sigma\exp(-\beta\mathcal{H}_0')\operatorname*{Tr}_{\sigma_r^z}\frac{e^{\beta J\sigma_r^z\sum_1^q\sigma_{r'}^z}-e^{-\beta J\sigma_r^z\sum_1^q\sigma_{r'}^z}}{2J\sigma_r^z\sum_1^q\sigma_{r'}^z}=2\beta Z_0^{-1}\operatorname*{Tr'}_\sigma\exp(-\beta\mathcal{H}_0')\frac{\sinh\left[\beta J\sum_1^q\sigma_{r'}^z\right]}{\beta J\sum_1^q\sigma_{r'}^z}\\&=2\beta Z_0^{-1}\operatorname*{Tr}_\sigma\exp(-\beta\mathcal{H}_0)\frac{\sinh\left[\beta J\sum_1^q\sigma_{r'}^z\right]}{\beta J\sum_1^q\sigma_{r'}^z}\,\frac{1}{\operatorname*{Tr}_{\sigma_r^z}e^{\beta J\sigma_r^z\sum_1^q\sigma_{r'}^z}}\\&=\beta Z_0^{-1}\operatorname*{Tr}_\sigma\exp(-\beta\mathcal{H}_0)\frac{\tanh\left[\beta J\sum_1^q\sigma_{r'}^z\right]}{\beta J\sum_1^q\sigma_{r'}^z}=\beta\left\langle\frac{\tanh\left[\beta J\sum_1^q\sigma_{r'}^z\right]}{\beta J\sum_1^q\sigma_{r'}^z}\right\rangle\ ,\end{aligned} \tag{2.16}$$

having used the definition of a canonical thermal average to begin and end the algebraic and partial-trace manipulations. Substituting (2.16) into (2.15) gives

$$\chi_{\perp}(T)=m^2\beta\sum_r\left\langle\frac{\tanh\left[\beta J\sum_1^q\sigma_{r'}^z\right]}{\beta J\sum_1^q\sigma_{r'}^z}\right\rangle, \qquad (2.17)$$

where the spin magnetic moment symbol m has now been explicitly entered. Concerning the notations used in (2.17), one is reminded that the inner summation variable r' as well as its upper value q are both functions of the outer summation variable r. The implications of $r'=r'(r)$, $q=q(r)$ will soon become clearer, particularly upon application to an irregular lattice having nonequivalent sites; for a *regular* lattice, however, the summation over all sites r in (2.17) merely enters a factor N (total number of lattice sites) and q is the lattice coordination number, giving the compact form of the original Fisher closed formula[1] as expected. As a generalization, the *basic formula* (2.17) for the isothermal zero-field perpendicular susceptibility $\chi_{\perp}(T)$ is *exact* for simple Ising models on regular or irregular lattices of arbitrary spatial dimensionality since no lattice symmetry or dimensionality arguments have been used in its derivation. The relatively simple structure of the basic formula (2.17) together with its wide applicability are noteworthy.

III. KAGOMÉ AND DECORATED-KAGOMÉ ISING MODELS AS EXAMPLES OF APPLICATION

The *kagomé* lattice (Japanese woven bamboo pattern) is a periodic array of equilateral triangles and regular hexagons (see Fig. 1) thus also called the 3-6 lattice.[7,8] The lattice is regular (all sites equivalent, all bonds equivalent) and may be termed "close packed" since it contains elementary polygons having an odd number of sides (viz., triangles). One recognizes that the kagomé lattice has the same coordination number 4 as the square lattice, the latter being "loose packed."

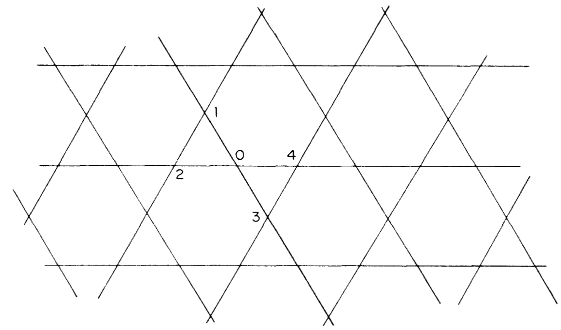

FIG. 1. The kagomé lattice where five sites are specifically enumerated, namely, the origin site and its four nearest-neighboring sites.

Applying the basic formula (2.17) to the kagomé Ising model, one obtains

$$\chi_{\perp}(T)=m^2\beta N\left\langle\frac{\tanh\left[Q\sum_1^4\sigma_{r'}^z\right]}{Q\sum_1^4\sigma_{r'}^z}\right\rangle, \qquad (3.1)$$

where the (dimensionless) interaction parameter $Q\equiv\beta J$. Using the site-labeling displayed in Fig. 1, the transcendental operator function appearing within the thermal average symbol can actually be expanded into a finite algebraic series since

$$\frac{\tanh[Q(\sigma_1^z+\sigma_2^z+\sigma_3^z+\sigma_4^z)]}{Q(\sigma_1^z+\sigma_2^z+\sigma_3^z+\sigma_4^z)}=A+B(\sigma_1^z\sigma_2^z+\sigma_1^z\sigma_3^z+\sigma_1^z\sigma_4^z+\sigma_2^z\sigma_3^z+\sigma_2^z\sigma_4^z+\sigma_3^z\sigma_4^z)+C\sigma_1^z\sigma_2^z\sigma_3^z\sigma_4^z, \qquad (3.2)$$

where

$$A=\frac{1}{8}\left[\frac{\tanh(4Q)}{4Q}+4\frac{\tanh(2Q)}{2Q}+3\right], \qquad (3.3a)$$

$$B=\frac{1}{8}\left[\frac{\tanh(4Q)}{4Q}-1\right], \qquad (3.3b)$$

$$C=\frac{1}{8}\left[\frac{\tanh(4Q)}{4Q}-4\frac{\tanh(2Q)}{2Q}+3\right], \qquad (3.3c)$$

use having been made of the facts that the left-hand side of (3.2) is an even function of its argument and any z-component Pauli spin operator σ_l^z (or corresponding Ising variable σ_l) satisfies $(\sigma_l^z)^{2n+1}=\sigma_l^z$, $(\sigma_l^z)^{2n}=1$, $n=0,1,2,\ldots$. The coefficient expressions (3.3) which depend only upon the (dimensionless) interaction parameter Q have been determined using again elementary spectral theory, i.e., considering all possible eigenvalue realizations of the operator forms in (3.2). Substituting (3.2) into (3.1) gives the dimensionless form

$$\frac{\chi_{\perp}(T)}{\chi_0}=4Q[A+2B(x_1+x_2+x_3)+Cx_5], \qquad (3.4)$$

where $\chi_0\equiv\chi_{\perp}(0)=Nm^2/4J$, the symmetry of the lattice has been recognized in the pair-wise equating of geometrically equivalent pair correlations, and the localized correlations are defined by

$$x_1=\langle 12\rangle,\quad x_2=\langle 14\rangle,\quad x_3=\langle 13\rangle,\quad x_5=\langle 1234\rangle, \qquad (3.5)$$

where, for simplicity of notation in (3.5), one has written in an obvious fashion only the numeric site labels within the thermal average symbols (see again Fig. 1).

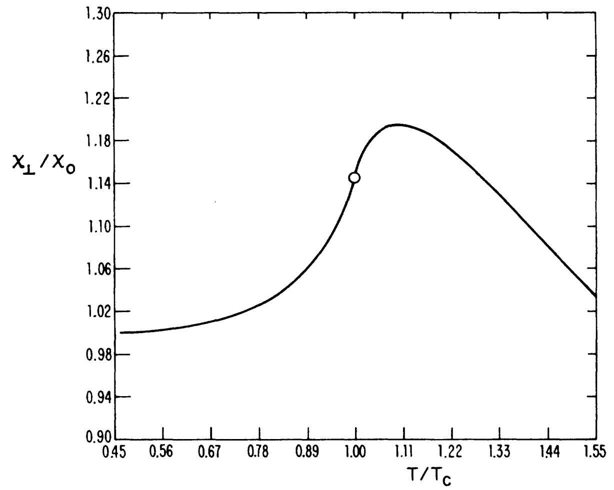

FIG. 2. Kagomé Ising model. Exact solution curve for the (reduced) transverse susceptibility $\chi_\perp(T)/\chi_0$ vs (reduced) temperature Q_c/Q $(=T/T_c)$ where $\chi_0=Nm^2/4J$; $Q_c=J/k_BT_c=\frac{1}{4}\ln(3+2\sqrt{3})=0.4665\ldots$. A vertical inflection point shown encircled exists at the critical temperature T_c. (Note the differing restricted ranges of the scales.)

Exact solutions for the ferromagnetic kagomé Ising model correlations (3.5) have recently[4] been obtained which together with the known interaction-dependent coefficients A,B,C [(3.3)] render the exact expression (3.4) for $\chi_\perp(T)/\chi_0$ explicitly calculable. Similar to the other three regular lattices, the resulting continuous curve in Fig. 2 for $\chi_\perp(T)/\chi_0$ versus T/T_c shows a weak (energy-type) singularity at the critical temperature T_c, where $\chi_\perp(T_c)/\chi_0=1.1426\ldots$ and a rounded maximum at $T_{\max}>T_c$ with the parameters of this maximum given by $\chi_\perp^{\max}/\chi_0=1.1945\ldots$ at $T_{\max}/T_c=1.0994\ldots$. Using corresponding reduced variables, these results on the kagomé lattice are numerically between those on the square and honeycomb lattices (given in Ref. 1) but very close actually to the former. This may be understood upon realization that $\chi_\perp(T)$ [as opposed to $\chi_\parallel(T)$] is a thermodynamic response function determined solely by correlations among the nearest-neighbor spins of an arbitrary spin and then recalling the fact that the kagomé and square-lattice structures each have the same coordination number 4.

In relation to the theory and results of the present work, one underscores that there exists an important axiom in statistical mechanics which requires the taking of the so-called *thermodynamic limit* ($\lim N\to\infty$, $V\to\infty$, where N/V is constant) and, to be safe, the thermodynamic limit should always be performed first, i.e., before all other limiting procedures in a statistical-mechanical theory. In the theory of phase transitions, the thermodynamic limit is clearly essential for obtaining mathematical singularities in the correlations and thermoscopic observables. For example, the correlations (3.5) which are substituted into (3.4) are those of the infinite lattice. In the present paper, for the convenience of retaining many of the same symbols and formulas found in the earlier references, the thermodynamic limit has not been explicitly written but rather is tacitly and indeed necessarily assumed. This choice of "lexicographical omission" causes no actual confusion in the context and, if desired, the incisive reader may insert the explicit thermodynamic limit notations where appropriate.

One next considers the lattice formed by the previous kagomé lattice supplemented with lattice points at the centers of all bonds (see Fig. 3). The resulting bond-decorated lattice is irregular since all sites are no longer equivalent, and is called the *decorated-kagomé* lattice. The decorated-kagomé Ising model ferromagnet is then defined by the Hamiltonian

$$\mathcal{H}_0=-\tilde{J}\sum_{\langle i,j\rangle}\sigma_i^z\mu_j^z \tag{3.6}$$

and the interaction energy[5] of the spin system with the transverse uniform, static, external magnetic field h_x is given by

$$\mathcal{H}_1=-h_x\left[\sum_i\sigma_i^x+\sum_j\mu_j^x\right]=-h_xM_x\ , \tag{3.7}$$

where σ_i^z,μ_j^z are z-component Pauli spin operators localized on the open-circled site i and solid-circled site j, respectively, $\sum_{\langle i,j\rangle}\cdots$ designates summation over all distinct nearest-neighbor pairs of lattice sites, $\tilde{J}>0$ is the strength parameter of the ferromagnetic interaction, and $M_x=\sum_i\sigma_i^x+\sum_j\mu_j^x$ is the x-component magnetic moment operator of the system.

The basic formula (2.17) for $\chi_\perp(T)$ can now be applied to the decorated-kagomé Ising model as the superposition expression

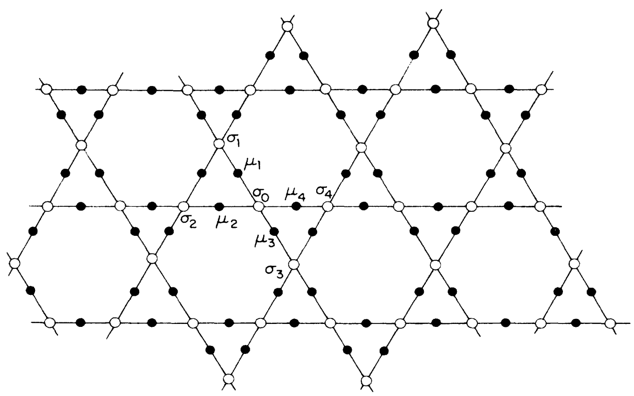

FIG. 3. The decorated-kagomé lattice where the open-circled sites are the original kagomé sites and the solid-circled sites are the new decoration sites. Nine site-localized Ising variables are specifically enumerated, namely, $\sigma_0,\sigma_1,\ldots,\sigma_4$ and $\mu_1,\ldots,\mu_4$.

$$\chi_{\perp}(T)=m^2\beta\left[\sum_{\substack{i\\ (\text{all}\ \circ\ \text{sites})}}\left\langle\frac{\tanh\left[P\sum_{1}^{4}\mu_{i'}^{z}\right]}{P\sum_{1}^{4}\mu_{i'}^{z}}\right\rangle+\sum_{\substack{j\\ (\text{all}\ \bullet\ \text{sites})}}\left\langle\frac{\tanh\left[P\sum_{1}^{2}\sigma_{j'}^{z}\right]}{P\sum_{1}^{2}\sigma_{j'}^{z}}\right\rangle\right] \tag{3.8}$$

with the (dimensionless) interaction parameter $P=\beta\tilde{J}$. Similar to the previous calculations, one next develops the transcendental functions of Ising-type operators within the thermal average symbols into finite algebraic series given by

$$\frac{\tanh[P(\mu_1^z+\mu_2^z+\mu_3^z+\mu_4^z)]}{P(\mu_1^z+\mu_2^z+\mu_3^z+\mu_4^z)}=A_1+B_1(\mu_1^z\mu_2^z+\mu_1^z\mu_3^z+\mu_1^z\mu_4^z+\mu_2^z\mu_3^z+\mu_2^z\mu_4^z+\mu_3^z\mu_4^z)+C_1\mu_1^z\mu_2^z\mu_3^z\mu_4^z\ , \tag{3.9}$$

where

$$A_1=\frac{1}{8}\left[\frac{\tanh(4P)}{4P}+4\frac{\tanh(2P)}{2P}+3\right]\ , \tag{3.10a}$$

$$B_1=\frac{1}{8}\left[\frac{\tanh(4P)}{4P}-1\right]\ , \tag{3.10b}$$

$$C_1=\frac{1}{8}\left[\frac{\tanh(4P)}{4P}-4\frac{\tanh(2P)}{2P}+3\right]\ , \tag{3.10c}$$

and

$$\frac{\tanh[P(\sigma_0^z+\sigma_1^z)]}{P(\sigma_0^z+\sigma_1^z)}=D_1+E_1\sigma_0^z\sigma_1^z\ , \tag{3.11}$$

where

$$D_1=\frac{1}{2}\left[\frac{\tanh(2P)}{2P}+1\right]\ , \tag{3.12a}$$

$$E_1=\frac{1}{2}\left[\frac{\tanh(2P)}{2P}-1\right]\ . \tag{3.12b}$$

The actual application of (3.8) also requires knowledge of the number of open- and solid-circled sites, $N_{\circ}$ and $N_{\bullet}$, respectively, which are easily counted since the total number of lattice sites $N=N_{\circ}+N_{\bullet}$ and $N_{\bullet}=2N_{\circ}$ together imply that

$$N_{\circ}=\tfrac{1}{3}N,\quad N_{\bullet}=\tfrac{2}{3}N\ . \tag{3.13}$$

Since all open-circled sites are equivalent, and likewise all solid-circled sites, the expression (3.8) for $\chi_{\perp}(T)$ together with (3.9), (3.11), and (3.13) yields

$$\begin{aligned}\chi_{\perp}(T)&=Nm^2\beta[\tfrac{1}{3}(A_1+B_1\langle\mu_1^z\mu_2^z+\mu_1^z\mu_3^z+\mu_1^z\mu_4^z+\mu_2^z\mu_3^z+\mu_2^z\mu_4^z+\mu_3^z\mu_4^z\rangle_{dk,P}+C_1\langle\mu_1^z\mu_2^z\mu_3^z\mu_4^z\rangle_{dk,P})+\tfrac{2}{3}(D_1+E_1\langle\sigma_0^z\sigma_1^z\rangle_{dk,P})]\\&=\tfrac{4}{5}\chi_0P[A_1+2B_1\langle\mu_1\mu_2+\mu_1\mu_3+\mu_1\mu_4\rangle_{dk,P}+C_1\langle\mu_1\mu_2\mu_3\mu_4\rangle_{dk,P}+2(D_1+E_1\langle\sigma_0\sigma_1\rangle_{dk,P})]\ ,\end{aligned} \tag{3.14}$$

where $\chi_0=\chi_{\perp}(0)=5Nm^2/12\tilde{J}$. In writing the last expression (3.14), the z superscripts have for simplicity been omitted by using the isomorphic Ising variables, the symmetry of the lattice has been recognized in the pair-wise equating of geometrically equivalent pair correlations, and the subscripts on all the thermal average symbols emphasize that these correlations are those of the decorated-kagomé (dk) Ising model having (dimensionless) interaction parameter P.

Using next an extended transformation theorem[4] of decoration-iteration type[9] (extended in the sense that the theorem applies beyond partition functions to multisite correlations), the above correlations on the decorated-kagomé Ising model having (dimensionless) interaction parameter P can be mapped upon linear combinations of correlations on the kagomé (k) Ising model having (dimensionless) interaction parameter Q, where P and Q are related [via (3.15g) below]. Specifically, using the notations depicted in Fig. 3, the theorem establishes for the present problem that

$$\begin{aligned}\langle\mu_1\mu_2\rangle_{dk,P}&=M^2\langle(\sigma_0+\sigma_1)(\sigma_0+\sigma_2)\rangle_{k,Q}\\&=M^2(1+3x_1)\ ,\end{aligned} \tag{3.15a}$$

$$\langle \mu_1\mu_3\rangle_{dk,P}=M^2\langle(\sigma_0+\sigma_1)(\sigma_0+\sigma_3)\rangle_{k,Q}$$
$$=M^2(1+2x_1+x_3)\ , \qquad (3.15b)$$
$$\langle \mu_1\mu_4\rangle_{dk,P}=M^2\langle(\sigma_0+\sigma_1)(\sigma_0+\sigma_4)\rangle_{k,Q}$$
$$=M^2(1+2x_1+x_2)\ , \qquad (3.15c)$$
$$\langle \mu_1\mu_2\mu_3\mu_4\rangle_{dk,P}=M^4\langle(\sigma_0+\sigma_1)(\sigma_0+\sigma_2)\times(\sigma_0+\sigma_3)(\sigma_0+\sigma_4)\rangle_{k,Q}$$
$$=M^4(1+6x_1+2x_2+2x_3+4x_4+x_5)\ , \qquad (3.15d)$$
$$\langle\sigma_0\sigma_1\rangle_{dk,P}=\langle\sigma_0\sigma_1\rangle_{k,Q}=x_1\ , \qquad (3.15e)$$

where

$$M=\tfrac{1}{2}(1-e^{-4Q})^{1/2} \qquad (3.15f)$$

and

$$e^{2Q}=\cosh(2P)\ . \qquad (3.15g)$$

In (3.15a)–(3.15e), the kagomé Ising model correlations are defined [consistently with (3.5)] by $x_1=\langle 12\rangle$, $x_2=\langle 14\rangle$, $x_3=\langle 13\rangle$, $x_4=\langle 0123\rangle$, and $x_5=\langle 1234\rangle$.

Since the kagomé Ising model correlations x_1,x_2,x_3,x_4,x_5 are known exactly,[4] the relations (3.15) are now substituted into (3.14) along with the known coefficients (3.10) and (3.12) thus enabling the exact solution $\chi_\perp(T)/\chi_0$ to be determined for the decorated-kagomé Ising model and the resulting curve is displayed in Fig. 4. An overall comparison of Figs. 2 and 4 reveals that the effect of the decoration spins (singly decorated bonds) is to diminish the reduced transverse susceptibility as a function of reduced temperature. A qualitatively new feature found in Fig. 4 is the appearance of a very gradual monotonically decreasing behavior of the curve at low temperatures until reaching a local minimum at $T_{\min}<T_c$ with the parameters of this very shallow (also asymmetric) minimum given by $\chi_\perp^{\min}/\chi_0=0.9970\ldots$ at $T_{\min}/T_c=0.6607\ldots$. The asymmetrical shape of this shallow minimum is not readily discernible to the eye in Fig. 4 with the scales chosen for the axes, but the numerical computer values in fact show that the higher-temperature side of the minimum is steeper than the broad low-temperature side. Similar to Fig. 2, the resulting continuous curve in Fig. 4 shows a weak (energy-type) singularity at the critical temperature T_c, where $\chi_\perp(T_c)/\chi_0=1.0711\ldots$ and a rounded maximum at $T_{\max}>T_c$ with the parameters of this maximum given by $\chi_\perp^{\max}/\chi_0=1.1086\ldots$ at $T_{\max}/T_c=1.1003\ldots$. Since all results are exact, both the qualitative and quantitative differences between Figs. 2 and 4 are attributable to the presence in the latter case of the decoration spins (singly decorated bonds).

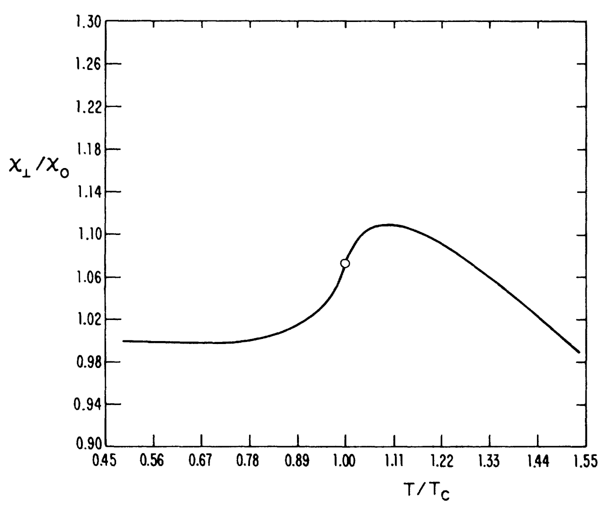

FIG. 4. Decorated-kagomé Ising model. Exact solution curve for the (reduced) transverse susceptibility $\chi_\perp(T)/\chi_0$ vs (reduced) temperature $P_c/P(=T/T_c)$, where $\chi_0=5Nm^2/12\tilde{J}$; $P_c=\tilde{J}/k_BT_c=\frac{1}{2}\ln[(3+2\sqrt{3})^{1/2}+(2+2\sqrt{3})^{1/2}]=0.7925\ldots$. A vertical inflection point shown encircled exists at the critical temperature T_c. (Note the differing restricted ranges of the scales.)

IV. SUMMARY AND CONCLUSIONS

The present theoretical investigations employ recently developed extended transformation theorems[4] which map unknown Ising multisite correlations upon linear combinations of those already known on other Ising models. Finding select even-number correlations on the kagomé and decorated-kagomé Ising models in this manner, the solutions are then substituted into exact analytical expressions for the zero-field perpendicular susceptibility $\chi_\perp(T)$ developed in large part by Horiguchi and Morita.[3]

Since there exist only four regular lattices in two dimensions, the present investigation upon the kagomé Ising model has succeeded in 'completing the list' of exact solutions for $\chi_\perp(T)$ of simple Ising models on regular planar lattice structures. The solution curve $\chi_\perp(T)/\chi_0$ versus T/T_c of the kagomé Ising model is numerically very close to that of the square Ising model which may be understood upon realization that the thermodynamic response function $\chi_\perp(T)$ [in contrast to $\chi_\parallel(T)$] is highly local in character and then recalling that both two-dimensional lattices have the same coordination number 4.

The present theory also directly advances systematic investigations of $\chi_\perp(T)$ for simple Ising models on *irregular* planar lattices. In particular, an exact solution is derived for $\chi_\perp(T)/\chi_0$ of the decorated-kagomé Ising model ferromagnet showing that the general effect of the decoration spins (singly decorated bonds) is to diminish the reduced transverse susceptibility as a function of reduced temperature although one still observes both a vertical inflection point (weak singularity of energy-type $\epsilon\ln\epsilon$, $\epsilon\equiv|T-T_c|/T_c$) at the critical temperature T_c and a rounded maximum at a temperature $T_{\max}>T_c$. As a qualitatively new feature, however, one notices a pronounced "flattening" of the curve at low temperatures relative to the previous kagomé Ising model. More precisely, there appears a slight monotonically decreasing behavior of the curve at low temperatures until reaching a very shallow (also asymmetric) local minimum at a temperature 34% below the critical temperature [one mentions that the existence of a shallow asymmetric local minimum for $\chi_{\perp}(T)/\chi_0$ at a temperature 14% below criticality was also found by Fisher[1] for an exactly soluble Ising model upon a plane antiferromagnetic superexchange lattice]. This local minimum phenomenon illustrates that findings upon irregular lattices cannot always be construed or inferred from those upon regular lattice structures. Although regular lattices have customarily been chosen for most calculations in statistical mechanics because the calculations are simplified and believed to contain most of the essential physics, one concludes by observing that, with the current 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 nature and which can now be more thoroughly investigated on site- and/or bond-irregular lattice structures with perhaps some special and diverse effects of their own to reveal.

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[5]The spin magnetic moment m ($\equiv g\mu_B/2$ in standard spectroscopic notation) actually appears here in the expressions for $\mathcal{H}_1 = -mh_x \sum_i \sigma_i^x$ and $M_x = m \sum_i \sigma_i^x$, but for present notational simplicity will be omitted and reentered appropriately at the conclusion of the calculations.

[6]See, for example, R. Abe, *Statistical Mechanics,* translated by Y. Takahashi (University of Tokyo Press, Tokyo, Japan, 1975).

[7]Examples of recent interest as realizations of the kagomé lattice include Frank-Kasper layered crystalline alloys, some of which show kagomé nets free of defects while in others the kagomé nets may contain "sequence faults." See, for example, F. C. Frank and J. S. Kasper, Acta Crystallogr. **11**, 184 (1958); **12**, 483 (1959); S. Sachdev and D. R. Nelson, Phys. Rev. B **32**, 1480 (1985). Also, iron atoms in jarosite-type materials are found to form kagomé layers in the crystal **C** plane. See M. G. Townsend, G. Longworth, and E. Rondant, Phys. Rev. B **33**, 4919 (1986).

[8]The deposition of monolayers upon various solid substrates is an active and advancing area of experimental and theoretical research. See, for example, M. Wortis, *Phases and Phase Transitions of Surfaces and Interfaces, in Fundamental Problems in Statistical Mechanics VI,* edited by E. G. D. Cohen (North-Holland, Amsterdam/New York, 1985), pp. 87–123; J. G. Dash, Physics Today **38**(12), 26 (1985), and references therein. The authors of the present paper are unaware of any fundamental reasons precluding the possibility of a kagomé configuration of atoms in select adlayer systems. One recalls that the kagomé lattice can in fact be constructed as the midpoints of all bonds of the honeycomb lattice, the latter lattice structure commonly found as a substrate and in various two-dimensional systems.

[9]For a review of decoration-iteration transformations upon Ising model partition functions, see, I. Syozi, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. I; for recent investigations upon decorated Ising models, see L. L. Gonçalves, Physica **133 A**, 345 (1985), and references therein.