Spontaneous magnetization and correlation functions in the Kagome lattice

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The spontaneous magnetization and correlation functions in the two-dimensional Kagome lattice are calculated. Because there are three spins in the unit cell, the ordered state is ferrimagnetic. Some features of the low-temperature transition are considered in detail. It is shown that, for a wide range of values of the interaction constants, there is a disordering temperature above the transition point, at which the spins with certain directions in the lattice are not correlated. The behavior of the system in virtual transition, i.e., when a small change in the interaction constants leads to the appearance of a low-temperature transition, is also discussed.

INTRODUCTION

It is well known that all two-dimensional Ising models display universal behavior[1] of the specific heat and the spontaneous moment near the transition point, independent of the lattice symmetry and the specific form of the spin-spin interaction. Together with these universal characteristics there exist others that are not universal, including, for instance, the transition temperature, the character of the saturation (with decreasing temperature) of the spontaneous moment, and the behavior of the correlation functions over a wider temperature range. Some features of the low-temperature transitions in the triangular lattice and in the model with non-nearest-neighbor interactions (NNNM)[3] have already been studied[2]. In the triangular lattice the region of universal behavior of the specific heat and the moment is extremely narrow, and the overall picture of the transition is that given by the Slater model[4].

In the present work the correlations and the spontaneous moment in the Kagome lattice (Fig. 1) are calculated. The unit cell of the lattice contains three spins, denoted by u, s, and t. Below the transition point the spontaneous moments of these spins, generally speaking, are not equal, and the ordering should be ferrimagnetic. In addition, the Kagome lattice has the property that in some range of values of the spin-spin interaction constants the transition occurs at low temperatures. It is therefore of interest to determine the features of the low-temperature transition in this model.

The calculation of the spontaneous moment is also of interest for another reason. The system of hydrogen bonds of the ferroelectric $NaH_3(SeO_3)_2$ (abbreviated STS), when expressed in terms of the Ising spin $\sigma = \pm 1$, has the form of a two-dimensional Kagome lattice[5]. True, in STS the non-nearest-neighbor interactions are significant, so that the results of an exact calculation of the Kagome lattice are not immediately applicable to sodium trihydroselenite. But since the cluster approximation[5,6] is used to describe the properties of STS as well as other hydrogen-containing ferroelectrics, it is interesting to compare the results of this method for the Kagome lattice with the exact results.

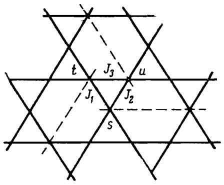

FIG. 1

It was shown in[2,7], using as example the NNNM and the triangular lattice, that in a rather wide range of values of the interaction constants the system possesses a so-called "disorder point". This phenomenon consists essentially of a change in the character of the correlations in the system at a certain temperature above the transition temperature. At this disordering temperature the specific heat does not have a singularity (long-range order does not appear in the system) but the correlation functions do have a singular point. In the Kagome lattice the disorder point is especially strong; for some directions in the lattice the correlations become zero at this point, and the correlation radius as a function of temperature has a cusp point.

In conclusion we shall discuss the character of the correlations in a virtual transition[2], i.e., when there is no phase transition in the system, but a small change in the interaction constants is sufficient to cause a low-temperature transition to appear.

SPONTANEOUS MOMENT

As is well known, the calculation of the partition function of the two-dimensional Ising model requires the diagonalization of a matrix, each element of which corresponds to a transition between neighboring spins along an interaction line. In the Kagome lattice this transition matrix is of twelfth order in the indices corresponding to different directions of leaving a site, since the unit cell of the lattice consists of three topologically inequivalent sites, each of which interacts with its four nearest neighbors. A calculation of the correlation function of two spins, lying along an interaction line in any one of the three possible directions, leads to very considerable difficulties. This is related to the high order (12th order) of the transition matrix and to the presence of two topologically different sites on the correlation line.

It is a much less difficult problem to find the correlation of spins along the directions shown by dotted lines in Fig. 1. Using the methods of Vdovichenko[8], the correlation function of the s-spins

$$G_s(r) = \langle s_0 s_r \rangle \qquad (1)$$

can be put into a form characteristic of an Ising lattice:

$$G_s(r)=\mathrm{Det}_r\, c_{k-l},\quad c_{k-l}=\int_0^{2\pi}\frac{d\omega}{2\pi}f_s(\omega)\,e^{i\omega(k-l)}. \tag{2}$$

Here $f_S(\omega)$ is specified by the formula

$$\begin{gathered}f_s(\omega)=g_s(\omega)/|g_s(\omega)|,\\ g_s(\omega)=z^2(1-x^2)^2(1-y^2)^2e^{2i\omega}\\ -[(1-x^4)(1-y^4)(1-z^4)-4xyz(1+z^2)(1-x^2)(1-y^2)]e^{i\omega}\\ +[2xy(1+z^2)-z(1+x^2)(1+y^2)]^2,\end{gathered} \tag{3}$$

and x, y, and z can be expressed in terms of the interaction constants as follows:

$$x=\mathrm{th}\,\beta J_1,\quad y=\mathrm{th}\,\beta J_2,$$
$$z=\mathrm{th}\,\beta J_3,\quad \beta=1/T.$$

The more significant points of this calculation are given in the Appendix. Obviously, from Eq. (3) we can obtain formulas similar to (1) for the correlation functions $G_t(r)$, of the t-spins, and $G_u(r)$, of the u-spins, by the corresponding cyclic exchanges of x, y, and z.

Setting $z = 0$ in Eq. (3) and carrying out a transformation with respect to the relations of x and y that is the inverse of the decoration transformation[9], we obtain a formula for the correlation along the diagonal in the square Ising lattice[1,10]. Given equal ferromagnetic constsnts $J_1 = J_2 = J_3 < 0$, we can calculate from Eqs. (2) and (3) the spontaneous moment obtained by Naya[9] by the successive application of the decoration transformation and the star-triangle transformation to the hexagonal lattice. In the general case of different interaction constants, this method does not lead to any result, due to the fact that the average values of the u-, s-, and t-spins, M_u, M_s, and M_t, do not agree.

Let us consider the most interesting region of antiferromagnetic values of the interaction constants: J_1, J_2, $J_3 > 0$. We assume in addition that $J_1 = J_2 \equiv J$. The free energy of the Kagome lattice was calculated by Kano and Naya[11], and in this case it can be written in the form

$$\begin{gathered}\beta F=-\frac{2}{3}\beta(\delta+J)-\frac{1}{6}\int_0^{2\pi}\!\!\int\frac{d\omega d\rho}{(2\pi)^2}\ln[1+6\alpha^4+\alpha^8+12\eta^2(1+\alpha^2)^2+8\eta^4\\ -4\eta(1-\alpha^2)^2(1+\alpha^2)(\cos\omega+\cos\rho)+4\cos(\omega+\rho)(\eta^2-\alpha^2)(1+\alpha^4-2\eta^2)];\\ \eta=e^{-2\beta\delta},\quad \alpha=e^{-2\beta J},\quad \delta=J-J_3.\end{gathered} \tag{4}$$

If $\delta > 0$, then at the temperature T_c specified by

$$(1-\alpha^2)^2-4\eta(1+\alpha^2)=0, \tag{5}$$

the system passes into an ordered state in which the u- and t-spins are antiparallel to the s-spins and parallel to one another. The total spontaneous moment of the lattice is nonzero.

In the given range of the interaction constants, we obtain from Eq. (3)

$$\begin{gathered}g_s(\omega)=4(\eta^2-\alpha^2)^2e^{2i\omega}-[4(\eta^2-\alpha^2)^2+(1+\alpha^4-2\eta^2)^2\\ -(1-\alpha^2)^4+16\eta^2(1+\alpha^2)^2]e^{i\omega}+(1+\alpha^4-2\eta^2)^2\end{gathered} \tag{6}$$

for the s-spins, and

$$\begin{gathered}g_t(\omega)=g_u(\omega)=4\eta^2(1-\alpha^2)^2e^{2i\omega}\\ -4\eta(1+\alpha^2)[(1+\alpha^2)^2+4\eta^2]e^{i\omega}+(1-\alpha^4)^2\end{gathered} \tag{7}$$

for the u- and t-spins. From Eqs. (2), (6), and (7) we find the average values of the spins, according to the Szego-Kac theorem[1,8,10], as the limit of $M^2 = \lim G(r)$ as $r \to \infty$:

$$M_t=M_u=[1-16\eta^4/(1+\alpha^2)^4]^{1/4}[1-16\eta^2(1+\alpha^2)^2/(1-\alpha^2)^4]^{1/8}, \tag{8}$$

$$M_s=\frac{1-\alpha^4}{1+\alpha^4-2\eta^2}M_t, \tag{9}$$

i.e., both M_S and M_t go to zero at the transition point like $|\tau|^{1/8}$, where $\tau = 1 - T/T_c$, but differ in magnitude.

When $J \gg \delta > 0$ ($J \sim J_3$) the transition is of the low-temperature type: $T_c \ll J$. In this case we can neglect the exponentially small terms $\sim\alpha$ in the exact formulas (4)—(9). Then

$$T_c\approx\delta/\ln 2, \tag{10}$$

and the specific heat per spin in the region $|\tau| \ll 1$ is

$$C\approx 2.1\ln(1/|\tau|).$$

Note that the coefficient of this logarithm is considerably larger than in the square Ising lattice, where it is approximately 0.5.

Figure 2 shows the behavior of the saturation of the s- and t-sublattice moments as functions of the reduced temperature. For purposes of comparison, the dotted line shows the behavior of the spontaneous moment of a square lattice.

It is clear physically that the smallness of T_c (see Eq. (10)) is related to the competition between the interactions in the triangle of u-, s-, and t-spins, i.e., the short-range correlations between spins are of major importance. The molecular field approximation provides a fair qualitative description of ordinary (not low-temperature) transitions in the Ising model; but in this case it does not give even an estimated order of magnitude for T_c. This is because the mean field approximation does not take into account nearest-neighbor correlations. Such a situation is characteristic of hydrogen-containing ferroelectrics of the order-disorder type[5,6]. We can extend this qualitative analogy by saying that the constant J has the meaning of the energy of a high-lying charged configuration, while δ represents the energy of a low-lying neutral configuration.

As we mentioned above, the transitions in these substances have been described with the help of the cluster approximation, in which the interaction between nearest neighbors is treated exactly and the influence of the remaining spins is treated as an average self-consistent field. In the Kagome lattice the simplest cluster is that consisting of the three neighboring spins: u, s, and t. Following the method of[5,6], we obtain

$$M_t^{(c)}=M_u^{(c)}=\{1-4\eta^2(1+\alpha^2)^2[(1-\alpha^2)^2-4\eta^2]^{-2}\}^{1/2}. \tag{11}$$

It is interesting to note that the exact relation (9) is satisfied in the cluster approximation. By neglecting the exponentially small terms of order α in Eq. (11), we obtain

$$T_c\approx 2\delta/\ln\left(\frac{4}{\sqrt{5}-1}\right).$$

This value differs from the exact result by $\approx$19%. The curve of $M_S^{(c)}$ is shown by the dot-dash line in Fig. 2; the curve of $M_t^{(c)}$ is not shown, in order not to overcomplicate the figure.

THE DISORDER POINT

Let us now consider in greater detail the character of the correlations in the lattice. From Eqs. (3), (6), and (7) we find that at the temperature (denoted T_d) specified by the equation

$$1+\alpha^2-2\eta=0, \tag{12}$$

the following relationship holds: $f_S(\omega) = f_t(\omega) = f_u(\omega) = -e^{-i\omega}$. Then the correlation functions $G_i(r)$ are ex-

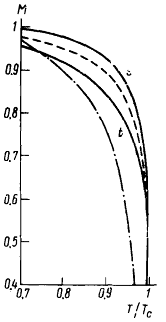

FIG. 2

actly zero, i.e., the spins are in neutral equilibrium with respect to one another. Equation (12) has a solution for T_d if $\delta > 0$, where $T_d > T_c$ always. Of course the correlations in other directions do not vanish. We can verify this by calculating the system energy from Eq. (4); it is expressed in terms of the correlations of the nearest neighbors along the bond lines.

The methods of calculating the asymptotic form of the correlation functions were developed in[10,12]. Using Wu's method, we find for $T > T_d$:

$$G(r)=\frac{\Delta}{2}\left[1-\frac{\Delta^2}{(\gamma_2-\gamma_1)^2}\right]^{1/4}\left(1-\frac{\Delta}{\gamma_2{}^2-1}\right)^{-1/2}e^{-r/\xi_+}k_+(r),$$
$$k_+(r)=\begin{cases}\pi^{-1/2}(r\Delta)^{-3/2}, & r\gg\max\{\xi_+,\Delta^{-1}\}\\ 1, & \xi_+\ll r\ll\Delta^{-1}\end{cases}\qquad(13)$$

Here $\Delta = 1 - \gamma_1\gamma_2$, the correlation radius $\xi_+ = (\ln\gamma_2)^{-1}$, and γ_1 and γ_2 are specified by Eq. (6) written in the form $g(\omega) = (e^{i\omega} - \gamma_1)(e^{i\omega} - \gamma_2)$. The general formula (13) is true for $G_s(r)$ and $G_t(r)$ if by γ_1 and γ_2 we mean the roots of $g_s(\omega)$ and $g_t(\omega)$ respectively. The inequality $\gamma_2 > 1 > \gamma_1 > 0$ holds over the entire temperature range $T > T_c$. From Eqs. (6) and (7) we obtain for Δ

$$\Delta_s=\frac{\eta^2(1-\alpha^2)^2}{(\eta^2-\alpha^2)^2}\Delta_t,\quad \Delta_t=1-\frac{(1+\alpha^2)^2}{4\eta^2}.\qquad(14)$$

Δ becomes zero at the point $T = T_d$.

In the range $T_c < T < T_d$ the correlation function has the form

$$G(r)=\frac{|\Delta|}{1-\Delta}\left[1-\frac{\Delta^2}{(\gamma_2-\gamma_1)^2}\right]^{1/4}\left(1+\frac{\Delta}{1-\Delta}\frac{1}{\gamma_1{}^{-1}-1}\right)^{1/2}e^{-r/\xi_-}k_-(r),$$
$$k_-(r)=\begin{cases}\dfrac{1}{\sqrt{\pi}}\left(r\dfrac{|\Delta|}{1-\Delta}\right)^{-1/2}, & r\gg\max\left\{\xi_-,\dfrac{1-\Delta}{|\Delta|}\right\}\\ 1, & \xi_-\ll r\ll\dfrac{1-\Delta}{|\Delta|}\end{cases}\qquad(15)$$

where $\xi_- = 1/\ln\gamma_1^{-1}$. In this temperature range $\Delta < 0$. Near T_c the correlation radius $\xi_-\alpha\tau^{-1}$, as in every two-dimensional Ising model. Below the transition point the correlations do not differ qualitatively from those in the square lattice[12].

Equations (13) and (15) show that at $T = T_d$ a change occurs in the short-range order. This phenomenon has been studied[2,7] in two two-dimensional models, the NNNM and the triangular lattice, and the corresponding temperature has been named by Stephenson the "disorder point." Except for the immediate neighborhood of T_d, the correlation function (15) has the same form as that in the square lattice above the transition, i.e., the coefficient before the exponent is proportional to $r^{-1/2}$. Also having the same appearance are the correlation functions in the NNNM and the triangular lattice in the range of temperatures above T_c and below T_d, so that below T_d the correlations have a universal form. At $T \geq T_d$ the behavior of the correlation functions changes and becomes strongly dependent on the lattice structure. But the physical nature of the disordering is the same in all these models, and is expanded by the above-mentioned competition between the interactions in the lattice. At high temperatures, $T \sim J$, the principal role is played by the direct interaction between nearest-neighbor spins. Thus, for instance, the neighboring spins u and t are antiparallel on the average. As the temperature drops the correlation radius increases, leading to an increase in the indirect interaction by way of other spins. The influence of the surrounding spins strongly renormalizes the original interaction constant. This is apparent from the fact that at low temperatures the effective interaction between the u- and t-spins has the opposite sign, since in the ordered phase they become parallel. At some intermediate temperature there can occur exact compensation of the original and "polarized" interactions in certain directions, and as a result the spins are no longer correlated. The disorder point appears most markedly in the Kagome lattice; in neither the NNNM nor the triangular lattice does the correlation function become zero for all distances[2,7]. It is also apparent from Eqs. (13) and (15) that, for the given directions, the correlation radius as a function of temperature has a deflection point at $T = T_d$, although it remains of order unity. However, the correlations in these directions provide no direct contribution to the energy, and the specific heat has no singularity at the disorder point.

When $\delta < 0$ the system has neither a phase transition nor a disorder point, and the asymptotic form (13) is correct at all temperatures. When $T \gg |\delta|$, $\eta \approx 1$ and the correlation functions of the s- and t-spins coincide. However, as the temperature drops $G_s(r)$ and $G_t(r)$ show different behavior. As $T \to 0$ the correlation radius of the s spins $\xi_s \approx \eta/2 \to \infty$, while $\xi_t \approx \ln^{-1}\eta = T/2|\delta| \to 0$. At the same time Eq. (14) shows that $\Delta_s \approx \eta^{-2} \to 0$, while $\Delta_t \approx 1 - 1/4\eta^2 \to 1$. At absolute zero temperature, $G_s(r) = G_t(r) = 0$. Unfortunately we do not know the correlation functions along the interaction lines, but from the form of G_s and G_t we can conclude that when $T \lesssim |\delta|$ there occurs one-dimensional ordering of the u- and t-spins along the line of the largest constant J_3, and the correlations between these one-dimensional chains are weakened. The thermodynamic behavior of the system corresponds to what was called in[2] a "virtual transition." The specific heat has a maximum at $T \sim |\delta|$, which becomes sharper as the ratio $|\delta|/J$ becomes smaller.

For the sake of argument we have considered above the region $J > 0$. The sign of J is not essential to the phenomena discussed above, the low-temperature and virtual transitions and the disorder point, but the constant J_3 must necessarily be antiferromagnetic. When $J < 0$ all the formulas remain the same if we make the exchange $\delta \to |J| - J_3$. The only difference is that in the ordered state all the spins are aligned parallel to one another.

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TABLE I

ν	ν': 1	2	3	4	5	6	7	8	9	10	11	12
1						$x\varepsilon^{-1}e_{-\rho}$		$x\varepsilon^2e_\rho$		$ye_{-\omega-\rho}$		
2						$xe_{-\rho}$				$y\varepsilon e_{-\omega-\rho}$		$y\varepsilon^{-2}e_{\omega+\rho}$
3						$x\varepsilon^2e_{-\rho}$		$x\varepsilon^{-1}e_\rho$				$ye_{\omega+\rho}$
4								xe_ρ		$y\varepsilon^{-2}e_{-\omega-\rho}$		$y\varepsilon e_{\omega+\rho}$
5		$x\varepsilon^{-2}e_{-\rho}$		$x\varepsilon e_\rho$					$ze_{-\omega}$			
6		$xe_{-\rho}$							$z\varepsilon^2e_{-\omega}$		$z\varepsilon^{-1}e_\omega$	
7		$x\varepsilon e_{-\rho}$		$x\varepsilon^{-2}e_\rho$							ze_ω	
8				xe_ρ					$z\varepsilon^{-1}e_{-\omega}$		$z\varepsilon^2e_\omega$	
9	$y\varepsilon^{-1}e_{-\omega-\rho}$		$y\varepsilon^2e_{\omega+\rho}$		$ze_{-\omega}$							
10	$ye_{-\omega-\rho}$				$z\varepsilon e_{-\omega}$		$z\varepsilon^{-2}e_\omega$					
11	$y\varepsilon^2e_{-\omega-\rho}$		$y\varepsilon^{-1}e_{\omega+\rho}$				ze_ω					
12			$ye_{\omega+\rho}$		$z\varepsilon^{-2}e_{-\omega}$		$z\varepsilon e_\omega$					

Here we use the notation $\exp(i\omega) = e_\omega$, $\exp(i\rho) = e_\rho$; the indices ν and ν' correspond to the different directions for leaving a lattice site:

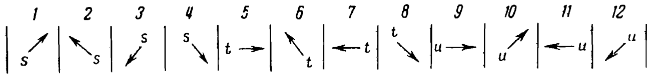

TABLE II

	$x \longleftrightarrow y$, $\varepsilon \to \varepsilon^{-1}$, $\rho \to -\omega-\rho$	$x \longleftrightarrow y$, $\varepsilon \to \varepsilon^{-1}$, $\omega \to -\omega$, $\rho \to \omega+\rho$	$\omega \to -\omega$, $\rho \to -\rho$		$x \longleftrightarrow y$, $\varepsilon \to \varepsilon^{-1}$, $\rho \to -\omega-\rho$	$x \longleftrightarrow y$, $\varepsilon \to \varepsilon^{-1}$, $\omega \to -\omega$, $\rho \to \omega+\rho$	$\omega \to -\omega$, $\rho \to -\rho$
$\lambda_{1,6}$	$-\lambda_{4,12}$	$-\lambda_{2,10}$	$\lambda_{3,8}$	$\lambda_{1,10}$	$-\lambda_{4,8}$	$-\lambda_{2,6}$	$\lambda_{3,12}$
$\lambda_{1,8}$	$-\lambda_{4,10}$	$-\lambda_{2,12}$	$\lambda_{3,6}$	$\lambda_{1,12}$	$-\lambda_{4,6}$	$-\lambda_{2,8}$	$\lambda_{3,10}$

APPENDIX

Following the method of Vdovichenko[7], the correlation function (1) can be written in the form

$$G(r)=\mathrm{Det}^{1/2}P_{l-l'}^{\mu,\mu'}. \tag{A.1}$$

The indices l and l' run over all values from 1 to r, and the indices μ and μ' from 1 to 14. The latter circumstance is due to the necessity of adding, to the twelve possible directions of leaving a lattice site along an interaction line, the two directions along the lines of the correlation to be calculated. By analogy with[7] we can verify that the determinant includes only the following matrix elements:

$$P_{l-l'}^{\mu,1}=-\int_0^{2\pi}\!\!\int\frac{d\omega d\rho}{(2\pi)^2}\exp[2i\omega(l-l'-1)]$$
$$\times\frac{\delta_{\mu,1}d(\omega,\rho)+\varepsilon p_{\mu,3}+\varepsilon^2p_{\mu,4}+\varepsilon^{-2}p_{\mu,5}+\varepsilon^{-1}p_{\mu,6}}{d(\omega,\rho)}, \tag{A.2}$$

$$P_{l-l'}^{\mu,2}=-\int_0^{2\pi}\!\!\int\frac{d\omega d\rho}{(2\pi)^2}\exp[2i\omega(l-l'+1)]$$
$$\times\frac{\delta_{\mu,2}d(\omega,\rho)+\varepsilon^{-2}p_{\mu,3}+\varepsilon^{-1}p_{\mu,4}+\varepsilon p_{\mu,5}+\varepsilon^2p_{\mu,6}}{d(\omega,\rho)} \tag{A.3}$$

In Eqs. (A.2) and (A.3) the index $\mu = 1, 2$; δ is the Kronecker symbol, $\epsilon = e^{i\pi/6}$, and

$$p_{\mu,\mu'}=(-1)^{\mu'-2}[xe^{-i\rho}(\delta_{\mu,1}\varepsilon^{-2}+\delta_{\mu,2}\varepsilon)\lambda_{\mu'-2,6}+xe^{i\rho}(\delta_{\mu,1}\varepsilon+\delta_{\mu,2}\varepsilon^{-2})\lambda_{\mu'-2,8}$$
$$+ye^{-i(\omega-\rho)}(\delta_{\mu,1}\varepsilon^{-1}+\delta_{\mu,2}\varepsilon^2)\lambda_{\mu'-2,10}+ye^{i(\omega+\rho)}(\delta_{\mu,1}\varepsilon^2+\delta_{\mu,2}\varepsilon^{-1})\lambda_{\mu'-2,12}], \tag{A.4}$$

where $\mu' = 3, 4, 5, 6$. $d(\omega, \rho)$ is the determinant, and $\lambda_{\nu,\nu'}$ are the minors of the twelfth-order matrix $\delta_{\nu,\nu'} - \Lambda_{\nu,\nu'}(\omega, \rho)$. The transition matrix $\Lambda_{\nu,\nu'}(\omega, \rho)$ is shown in Table I.

Thus there are sixteen eleventh-order minors $\lambda_{\nu,\nu'}$ included in the matrix elements $P_{1-1'}^{\mu,1}$ and $P_{1-1'}^{\mu,2}$. Of these, four are independent. If we choose the four independent minors to be $\lambda_{1,6}$, $\lambda_{1,8}$, $\lambda_{1,10}$, and $\lambda_{1,12}$, then the remaining minors can be obtained from them by replacement of variables as shown in Table II. These relationships follow from the symmetry of the Kagome lattice and may be verified by observation.

After the cumbersome calculation of the minors and their substitution in Eqs. (A.2)—(A.4), we find that $P_{l-l'}^{1,2} = P_{l-l'}^{2,1} = 0$ and $P_{l-l'}^{1,1} = P_{l-l'}^{2,2}$. Then

$$\mathrm{Det}^{1/2}P_{l-l'}^{\mu,\mu'}=\mathrm{Det}\,P_{l-l'}^{1,1}.$$

By performing the integration over ρ in $P_{l-l'}^{1,1}$ we arrive at Eqs. (2) and (3), where we have used the notation $P_{l-l'}^{1,1} = c_{l-l'}$.

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