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Initial Perpendicular Isothermal Susceptibility Formulas for the Transverse General-Spin Ising and Blume–Capel Models

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Using a Kubo formula and the Suzuki identities, expressions are derived for the initial perpendicular susceptibilities $\chi_\perp$ of the transverse spin-S Ising and spin-S Blume–Capel models on regular and irregular lattices. $\chi_\perp$ is given in terms of the thermal average of a function of the peripheral sum $O_i = \sum_j J_{ij} S_j$, where coupling to distant neighbors may be included, as well as arbitrary local parallel magnetic fields h_j. For the Ising model on a Bravais lattice, e.g., the susceptibility is given by

$$\chi_\perp = Nm^2 S^{-2} \langle B_S(\beta[O_i + h_i])/[O_i + h_i] \rangle$$

where B_S is the Brillouin function. For $S = \frac{1}{2}$, the formula of Fisher and the results of Horiguchi and Morita are regained. A connection is made with the general-spin work of Essam and Garelick.

KEY WORDS: Perpendicular susceptibility; isothermal susceptibility; Ising model; Blume–Capel model.

1. INTRODUCTION

A formula for the perpendicular susceptibility of the transverse spin-$\frac{1}{2}$ Ising model, in terms of multispin correlation functions, was first given by Fisher,[1] using a combination of graph-theoretic considerations and straightforward matrix analysis. It was applied by him to the quadratic, honeycomb and Bethe lattices, and by Stephenson[2] to the triangular lattice. As derived, the formula held only for regular lattices. It was extended,

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using the Kubo[3] formalism, to cover irregular lattices by Horiguchi and Morita,[4] with application by Barry[5] to the Kagomé and the decorated Kagomé lattices. For the three-dimensional lattices, where the relevant multispin correlations are not known analytically, this formula has not been used. Rather, $\chi_\perp$ has been studied by analysis of high- and low-temperature series expansion methods[6,7] and by correlated effective field methods.[8]

Recently, closed-form theories have been developed[9–14] that give the required multispin correlation functions at the critical point (and also, in principle, away from T_c) to a relatively high degree of accuracy[9] (namely, within 1 or 2% of available series and Monte Carlo calculation results) and with relatively little cost in computation time, when the following Ising systems are considered: (i) those for spin $\frac{1}{2}$[9] and spin 1,[10] (ii) for spin $S>1$,[11] (iii) pair interactions, with further neighbor bonds,[12] (iv) on lattices of $d\geqslant 3$ spatial dimensions,[13] and (v) with quartet as well as pair interactions.[14] It is of interest, therefore, to develop formulas that will be of use in calculating $\chi_\perp$ for all these systems, as well as for more general systems that are in principle capable of treatment by similar closed-form methods.

In the following, starting from the well-known Kubo formula[3] and using a Suzuki identity,[15] the perpendicular susceptibility formula is derived in a simple way for the simplest spin-S transverse Ising system. This is done in order to illustrate the basic elements of our approach. Several immediate generalizations to other, more complicated, Ising models are then indicated. To display its versatility, the approach is used finally to consider the transverse Blume–Capel[16,17] model generalized to spin S.

2. THEORY; ISING MODEL

2.1. Bravais Lattice

We start with the simple spin-S transverse Ising model Hamiltonian

$$\begin{aligned} H_T &= H - mS^{-1}H_x \sum_j S_j^x \\ H &= -\frac{1}{2}\sum_{j,k} J_{jk} S_j^z S_k^z \end{aligned} \tag{2.1}$$

where J_{jk} is J or 0, depending on whether or not j and k are nearest neighbors, j and k label the N lattice sites of a Bravais lattice, and H_x is the external magnetic field, taken to be in the x direction. Each S_j^z may take on the values $-S$, $-S+1$,..., $+S$. In terms of this Hamiltonian, the initial

(i.e., as $H_x \to 0$) perpendicular susceptibility is given by Kubo[3] (see also Betts[18] for a particularly clear derivation) as

$$\chi_\perp = (\partial \langle M_\perp \rangle / \partial H_x)_{H_x \to 0}$$
$$= \int_0^\beta \langle \exp(\lambda H)\, M_\perp \exp(-\lambda H) M_\perp \rangle \, d\lambda \tag{2.2}$$

where $\beta = 1/k_B T$,

$$M_\perp = mS^{-1} S_x \equiv mS^{-1} \sum_j S_j^x \tag{2.3}$$

and the thermal average is given by

$$\langle \cdots \rangle = Z^{-1} \operatorname{Tr}[\exp(-\beta H) \cdots] \tag{2.4}$$

with

$$Z = \operatorname{Tr}[\exp(-\beta H)] \tag{2.5}$$

A term $-\beta \langle M_\perp \rangle^2$ originally in (2.2) has been omitted; for H axial it vanishes. As all sites are equivalent on a Bravais lattice, the integrand I of (2.2) becomes

$$I = C' N \langle \exp(\lambda H) S_i^x \exp(-\lambda H) S^x \rangle \tag{2.6}$$

where i is any chosen lattice site and $C' = m^2 S^{-2}$. Further, as H is invariant to rotation about the z axis in the subspace of any spin i, the only surviving term of (2.6) when the sum (2.3) of S^x is inserted is

$$I = C' N \langle \exp(\lambda H) S_i^x \exp(-\lambda H) S_i^x \rangle \tag{2.7}$$

Using the ladder operators $S_i^\pm = S_i^x \pm i S_i^y$, so that $S_i^x = (S_i^+ + S_i^-)/2$, one has

$$I = CN \langle \exp(\lambda H) S_i^+ \exp(-\lambda H) S_i^- \rangle + \text{term with } S_i^- \leftrightarrow S_i^+ \tag{2.8}$$

where $C = m^2 S^{-2}/4$. The cross terms have vanished due to the fact that, e.g., a double S_i^+ changes any eigenfunction of S_i^z into one with an eigenvalue increased by two units, which is orthogonal to the original one (while H is diagonal in S_i^z). The term with S_i^- and S_i^+ interchanged gives, when integrated, a result equivalent to that of the written term; this can be seen by changing the integration variable from λ to $\lambda' = \beta - \lambda$ and using the cyclic property of the trace. One now writes

$$\exp(\lambda H) S_i^+ \exp(-\lambda H) = \exp(-\lambda S_i^z O_i) S_i^+ \exp(\lambda S_i^z O_i)$$
$$= \exp(-\lambda O_i) S_i^+ \tag{2.9}$$

where $O_i = \sum_j J_{ij} S_j^z$ and where in the first step all operators in H not involving the site i are commuted through the S_i^+, and in the second step

the commutation relation $[S_i^+, S_i^z] = -S_i^+$ is used. Substituting into (2.8) and then (2.2), interchanging the integral and the trace, and performing the integration, we have

$$\chi_\perp = -2CNZ^{-1} \operatorname{Tr} \left\{ \exp(-\beta H) \frac{\exp(-\beta O_i) - 1}{O_i} S_i^+ S_i^- \right\} \tag{2.10}$$

[The question of the validity of (2.10) arises here for the situation where O_i has the eigenvalue zero. In this case the λ integration would give $-\beta$ instead of the $[\exp(-\beta O_i) - 1]/O_i$ of (2.10). But $-\beta$ is simply the limit of the latter expression as $O_i \to 0$ *formally*. Thus, (2.10) may be retained even in this case with the understanding that when O_i has the eigenvalue zero, the limit is to be taken.] Equation (2.9) is now used in reverse, with λ replaced by β, to obtain (2.10) in the form (noting that O_i commutes with all the operators)

$$\begin{aligned} \chi_\perp &= -2CNZ^{-1} \operatorname{Tr}\{(O_i)^{-1}[S_i^+ \exp(-\beta H) S_i^- - \exp(-\beta H) S_i^+ S_i^-]\} \\ &= 2CN\langle [S_i^+, S_i^-]/O_i \rangle \\ &= 4CN\langle S_i^z/O_i \rangle \end{aligned} \tag{2.11}$$

where an $\exp(-\beta H)$ has canceled against an $\exp(\beta H)$, and the cyclic invariance property of the trace, $\operatorname{Tr} AB = \operatorname{Tr} BA$, has been used. The spin-S Ising model Suzuki[15] identity

$$\langle \{\bar{i}\} S_i^z \rangle = \langle \{\bar{i}\} B_S(\beta O_i) \rangle \tag{2.12}$$

where $\{\bar{i}\}$ is any function of any spins not involving S_i^z, is now invoked to obtain the perpendicular susceptibility in the form

$$\chi_\perp = Nm^2 S^{-2} \langle B_S(\beta O_i)/O_i \rangle \tag{2.13}$$

B_S is the Brillouin function given by

$$B_S(x) = (S + \tfrac{1}{2}) \coth[(S + \tfrac{1}{2})x] - \tfrac{1}{2} \coth(\tfrac{1}{2}x)$$

For $S = \frac{1}{2}$, one uses $B_{1/2}(x) = \frac{1}{2} \tanh \frac{1}{2}x$ in (2.13) to recapture the formula derived by Fisher [Ref. 1, (4.2) combined with (4.9) and (4.10)].

2.2. Generalizations

If the Zeeman term $-\sum_i h_i S_i^z$ [with $h_i = mS^{-1}(H_z)_i$] is added to H, thereby allowing the magnetic field to have a local z component, the derivation goes through as before, with O_i replaced by $O_i + h_i$:

$$\chi_\perp = Nm^2 S^{-2} \langle B_S(\beta(O_i + h_i))/(O_i + h_i) \rangle \tag{2.14}$$

Nowhere in the derivation was the nearest neighbor property of the J_{ij} used or the space dimensionality of the lattice, so that (2.14) holds for any range of coupling and any dimensionality. If the spins are distributed on a regular lattice which is not necessarily Bravais, so that all sites are equivalent for the purposes of this calculation, formula (2.14) is seen to hold with N now being the total number of spins in the system. If the spins are distributed on an irregular lattice, which can be described as a Bravais lattice with a basis, then with the notation $r = 1, 2, ..., n$ labeling the spins on the basis sites within a single Bravais cell labeled by i, (2.14) is seen to generalize to

$$\chi_\perp = Nm^2 S^{-2} \sum_r \langle B_S(\beta(O_{i,r} + h_{i,r}))/(O_{i,r} + h_{i,r}) \rangle \tag{2.15}$$

where N is the total number of Bravais lattice sites.

3. BLUME–CAPEL MODEL

For this model[16,17] the Hamiltonian is

$$H_{\text{B-C}} = H_{\text{Ising}} + \Delta (S_i^z)^2 \tag{3.1}$$

where Δ is a splitting parameter. Using the general formula

$$f(S_i^z) S_i^+ = S_i^+ f(S_i^z + 1) \tag{3.2}$$

for any function f, one proceeds through the stages of Section 2.1 to obtain, instead of (2.11),

$$\begin{aligned} \chi_\perp = & -2CNZ^{-1} \operatorname{Tr}\{(O_i - 2\Delta S_i^z + \Delta)^{-1} [S_i^+ \exp(-\beta H) \\ & - \exp(-\beta H) S_i^+] S_i^-\} \end{aligned}$$

Using (3.2) again for the first term,

$$\begin{aligned} \chi_\perp = & -2CNZ^{-1} \operatorname{Tr}\{[S_i^+ (O_i - 2\Delta S_i^z - \Delta)^{-1} \exp(-\beta H) \\ & - (O_i - 2\Delta S_i^z + \Delta)^{-1} \exp(-\beta H) S_i^+] S_i^-\} \end{aligned} \tag{3.3}$$

and again using the cyclic invariance property of the trace,

$$\chi_\perp = -2CN \langle (O_i - 2\Delta S_i^z - \Delta)^{-1} S_i^- S_i^+ - (O_i - 2\Delta S_i^z + \Delta)^{-1} S_i^+ S_i^- \rangle$$

or

$$\chi_\perp = \frac{1}{2} Nm^2 S^{-2} \left\langle \frac{S(S+1) - (S_i^z)^2 + S_i^z}{O_i - 2\Delta S_i^z + \Delta} - \frac{S(S+1) - (S_i^z)^2 - S_i^z}{O_i - 2\Delta S_i^z - \Delta} \right\rangle \tag{3.4}$$

where the well-known formulas for $S_i^+ S_i^-$ and $S_i^- S_i^+$ have been invoked. Relation (3.4) reduces to (2.11) in the limit $\Delta \to 0$. Now, to obtain (3.4) as a function of the O_i alone [as in (2.13)], one simply does a partial trace as in Suzuki,[15] i.e.,

$$\langle f(S_i^z)\rangle = \Bigg\langle \sum_{S_i^z=-S}^{+S} \exp\{\beta[S_i^z O_i - \Delta(S_i^z)^2]\} \times f(S_i^z) \Big/ \sum_{S_i^z=-S}^{S} \exp\{\beta[S_i^z O_i - \Delta(S_i^z)^2]\} \Bigg\rangle \tag{3.5}$$

Equation (3.5) holds even when O_i appears (as a parameter) in f, as it does in the present case. In practice, there is no need to attempt to reduce (3.5) to known simple functions.

It is noted that (3.4) holds for general spin S; a formula is thus obtained for the general S Blume–Capel model, originally defined for spin 1.

4. CONCLUDING REMARKS

It is clear from the above derivations that the same method can be used to derive formulas for the initial perpendicular susceptibility for even more general models, including those with $\sum_{n=3} \Delta_n (S_i^z)^n$ added to the Hamiltonian (the Δ_n being additional splitting parameters). In the Appendix, it is shown how one may obtain our general Ising formula (2.14) from the spin-S results of Essam and Garelick.[19]

APPENDIX

Essam and Garelick[19] studied the difference between the static limit of the frequency-dependent transverse susceptibility and the isothermal susceptibility, for the spin-S Ising model. Combining their equations (5.15) and (5.25), we have (in our notation) what would be *their* expression for the isothermal susceptibility:

$$\chi_\perp = \frac{Nm^2}{S^2} \sum_{\substack{r \\ \omega_r \neq 0}} \frac{\langle P_r S_i^z \rangle}{\omega_r} + Nm^2 \beta \frac{S+1}{3S} \langle P_0 \rangle \tag{A1}$$

where the ω_r are the eigenvalues of O_i, P_r is the projection operator that projects onto the subspace corresponding to ω_r, and P_0 is the projection operator corresponding to $\omega_r = 0$. Now, since

$$B_S(x) = xS(S+1)/3 + O(x^3) \tag{A2}$$

for small x, we have

$$[Nm^2\beta(S+1)/3S]\langle P_0\rangle = (Nm^2/S^2)\langle P_0 B_S(\beta O_i)/O_i\rangle \tag{A3}$$

At the same time, the Suzuki identity[15] gives

$$\langle P_r S_i^z/\omega_r\rangle = \langle P_r B_S(\beta O_i)/O_i\rangle \tag{A4}$$

With (A4) and (A3) in (A1),

$$\chi_\perp = (Nm^2/S^2)\sum_r \langle P_r B_S(\beta O_i)/O_i\rangle \tag{A5}$$

where the sum over r is now unrestricted, so that $\sum_r P_r = 1$ may be used to obtain (2.13). In reality the ω_r were originally defined as the eigenvalues of $O_i + h_i$ (for simplicity h_i was set equal to zero above), so that (2.14) is obtained in the same way.

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