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Exact solution for the inelastic neutron scattering from an anisotropic honeycomb Ising magnet

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Abstract. We consider an anisotropic Ising model ferromagnet on the honeycomb lattice, having nearest-neighbour pairwise interactions J, $\theta J > 0$ along the oblique and horizontal lattice axes, respectively, with $\theta > 0$ being an anisotropy parameter. Since the Hamiltonian contains solely z-component (longitudinal) Pauli spin operators, the dynamics in the Ising model evolves only for the non-ordering (transverse) spin degrees of freedom. An exact solution is calculated for the inelastic neutron scattering function $S^{xx}(q, \omega) = \Sigma_n A_n(T, \theta)\, \delta(\omega - \omega_n(\theta))$, $n = \pm 3, \pm 2, \pm 1$, which depends upon the frequency ω, temperature T and anisotropy θ. The discrete energy transfers $\hbar\omega_n(\theta)$ are independent of temperature, vary linearly with θ and possess degeneracies for certain integral values of θ. The scattering amplitudes (intensities/site) $A_n(T, \theta)$ of the Dirac δ-functions exhibit, for fixed θ, such behaviours as rounded maxima, crossing points, and weak energy-type singularities at the critical temperature $T_c(\theta)$. At criticality, the 'spin wave mode' scattering amplitude versus anisotropy displays a shallow asymmetric minimum at $\theta = 1$. Compared with the existence of only four inelastic scattering modes in the isotropic ($\theta = 1$) case, the present six modes illustrate the partial lifting of essential degeneracies. Some similar results may be inferred for the more general case having two anisotropy parameters and eight modes.

1. Introduction

Neutron scattering spectroscopy is a particularly valuable and versatile method for investigating condensed matter [1]. The neutrons thermalized by the moderating light or heavy water in a research reactor are abundant in number and well suited in their wavelengths to probe various physical properties on an atomic length scale (~1 Å). Also, since the energies of the incident thermal neutrons in a scattering experiment are typically of order $k_B T_M$ where T_M is the moderator temperature, whenever such neutrons are used to investigate materials for energy levels of this magnitude ($\sim 10^{-2}$ eV), the fractional change in energy for a scattering event will be large and thus easy to measure.

Two-dimensional ($d = 2$) magnetic systems [2], especially in alliance with lattice-statistical models, have been very important in the studies of phase transitions, critical and multicritical phenomena. Interest has intensified in recent years because of the $d = 2$ nature of magnetic excitations in high-temperature superconductors. The study of excitations is in itself a rich field. In these investigations, exactly soluble models can be useful both as guides to the behaviours in more complex systems and because very often the model itself is realizable in a physical system. For example, the layered magnetic compounds K_2CoF_4 and Rb_2CoF_4 behave as $d = 2$ Ising models [3]. In general, the best

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way to probe the magnetic excitation spectrum is by inelastic neutron scattering. Apart from factors related to the Fourier transform of the atomic magnetization density and the spin polarization of the scattered neutron, neutron scattering provides a direct measure of the dynamical spin correlation function $S^{\alpha\alpha}(q, \omega)$, $\alpha = x, y, z$.

The inelastic neutron scattering from an isotropic square Ising magnet was previously derived exactly by Allan and Betts [4], and the results graphed at a few select temperatures including the critical temperature. The present paper determines the exact solution for the transverse dynamical spin correlation function $S^{xx}(q, \omega)$ of an anisotropic Ising ferromagnet on the $d = 2$ honeycomb lattice, at all temperatures and arbitrary values of the anisotropy. In general, an Ising model is incomplete for describing such dynamical effects in actual physical systems since $S^{xx}(q, \omega)$ of an Ising model exhibits neither dependence on wave-vector q, nor line-widths $\Delta\omega$ in energy, which can be understood rather intuitively as follows. The elementary excitations of an Ising model magnet, being 'individual spin flips', are most highly localized in the lattice configuration space, i.e. there are no collective-type modes. Consequently, the corresponding momentum transfer q-distribution is *uniform*. Also, since the local z-magnetization operator commutes with the Ising system total Hamiltonian, it is a constant of motion, and an Ising spin after being 'flipped' by a neutron thus takes an infinitely long time to recover its original orientation (relaxation time $\tau = \infty$). Because the excitations are infinitely long-lived, any associated line-width $\Delta\omega \propto \tau^{-1}$ is vanishingly small causing *sharpness* of energy (namely, Dirac δ-functions) to emerge in the neutron scattering results. Of course, in a real magnetic crystal, additional transverse spin couplings and long-range forces such as dipole–dipole and spin–lattice interactions would induce q-dependencies and finite line-widths $\Delta\omega$ in the resonances.

These significant limitations notwithstanding, since all the required localized correlations are exactly calculable in the present case of an anisotropic honeycomb Ising model ferromagnet, the locations and amplitudes of the δ-functions in energy are obtained exactly as functions of temperature and anisotropy, reflecting the probabilities for the incident neutrons to encounter highly localized 'star' clusters of specific spin configurations. These exact solution curves of the scattering intensities for all temperatures and arbitrary values of the anisotropy are evidently (and perhaps surprisingly) the first to appear explicitly in the literature, thereby enabling inspection of such features as rounded extrema, crossing points and weak (energy-type) singularities at criticality, where the locations and shapes of these features vary with anisotropy. Moreover, it is observed that each of the localized static correlations comprising the scattering intensities may be experimentally accessible.

2. Anisotropic honeycomb Ising magnet

The honeycomb lattice structure is a $d = 2$ periodic array of regular hexagons (see figure 1). The honeycomb pattern [5] is one of the most frequently occurring $d = 2$ designs in nature (and art), with examples including the prototype beeswax honeycomb, the retinal pigment of one's eye, Indian corn (maize), skeletal remains of marine life, geological arrangements of suddenly cooled magma, crystallographic forms (basal plane of graphite, etc) and a plethora of other illustrations some of which, like the brick-wall lattice, are topologically equivalent to the honeycomb lattice.

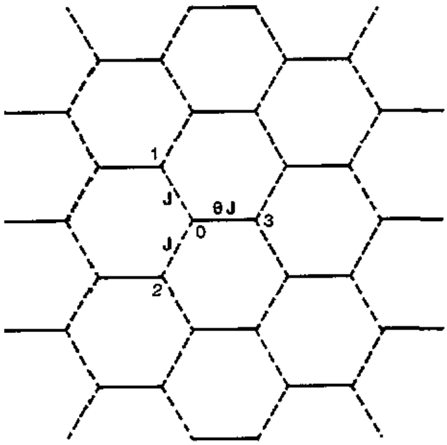

Figure 1. The honeycomb lattice where four sites are specifically enumerated, namely, an origin site and its three nearest-neighbouring sites. The Ising interactions along the oblique (dashed) bonds have strength J whereas those along the horizontal (solid) bonds have strength θJ.

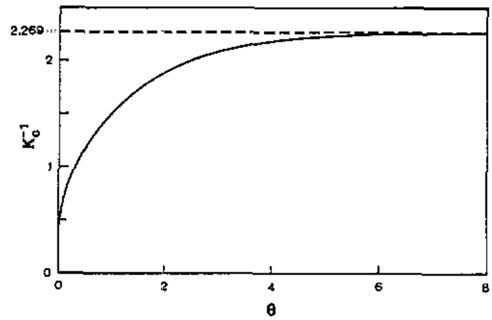

Figure 2. The (reduced) critical temperature K_c^{-1} ($\equiv k_B T_c/J$) versus the anisotropy parameter θ. As $\theta \to \infty$, $K_c^{-1} \to 2/\ln(1+\sqrt{2}) = 2.269\,18\ldots$ (isotropic square Ising ferromagnet).

One now defines an anisotropic honeycomb Ising model ferromagnet on such a lattice of N sites as the classical Ising Hamiltonian

$$\mathcal{H}_{cl} = -J \sum_{\langle l,k\rangle_o} \sigma_l \sigma_k - \theta J \sum_{\langle l,k\rangle_h} \sigma_l \sigma_k \tag{2.1}$$

where each site-localized Ising variable $\sigma_p = \pm 1$, $\Sigma_{\langle l,k\rangle_o} \ldots$ indicates summation over all distinct nearest-neighbour pairs of lattice sites along the *oblique* lattice axes with $\Sigma_{\langle l,k\rangle_h} \ldots$ being similarly defined along the *horizontal* lattice axis, and $J > 0$ is a strength parameter of the ferromagnetic interaction with $\theta > 0$ being an anisotropy parameter.

Since the partition function of the Ising model (2.1) is known exactly [6], various thermodynamic properties of the system can be found exactly in the standard manner from the first and second derivatives of the characteristic free energy. For present purposes, the dependence of the critical temperature upon anisotropy, $T_c = T_c(\theta)$, can be determined implicitly from the relation [6]

$$\frac{1}{2K_c} \ln\left(\frac{e^{-4K_c} - 2e^{-2K_c} - 1}{e^{-4K_c} + 2e^{-2K_c} - 1}\right) = \theta \tag{2.2}$$

where $K_c \equiv J/k_B T_c$ with k_B being the Boltzmann constant and T_c the critical absolute temperature (see figure 2).

Specializations in the thermostatistical behaviour of the Ising model (2.1) include: (a) $\theta \to 0$: independent Ising chains; (b) $\theta = 1$: isotropic honeycomb Ising ferromagnet; (c) $\theta \to \infty$: isotropic square Ising ferromagnet; (d) $\theta \to \infty$, $J \to 0$, $\theta J =$ constant: independent Ising dimers. Some considerations involving a more general anisotropic case having different couplings along each of the three crystal axes will be given at the end of the paper.

The Ising σ-variables are isomorphic to the corresponding z-component Pauli spin operators σ_l^z, the latter operators being used for the quantal version of the classical model (2.1). As will be seen shortly, the quantal Ising model is actually required for treating the inelastic neutron scattering problem.

3. Inelastic neutron scattering function

Theoretical investigation of the inelastic neutron scattering double-differential cross-section entails evaluation of the function [1, 2, 4]

$$\mathcal{S}^{xx}(\boldsymbol{q}, \omega) = \sum_n \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}t \sum_m \exp[\mathrm{i}\boldsymbol{q} \cdot (\boldsymbol{R}_m - \boldsymbol{R}_n) - \mathrm{i}\omega t] \langle \sigma_n^x \sigma_m^x(t) \rangle \qquad (3.1)$$

where $\boldsymbol{R}_m, \boldsymbol{R}_n$ are the lattice position vectors of sites m and n, respectively. The summand of Σ_n is the temporal-lattice Fourier transform of the two-time, two-site transverse spin correlation $\langle \sigma_n^x \sigma_m^x(t) \rangle$ where $\boldsymbol{q} = \boldsymbol{k}_{\mathrm{in}} - \boldsymbol{k}_{\mathrm{fin}}$ is the difference between the initial and final wave vectors of the neutron, and $\hbar\omega = \hbar^2(k_{\mathrm{in}}^2 - k_{\mathrm{fin}}^2)/2m_0$ is the energy transferred from the neutron to the spin system with m_0 being the neutron mass and $2\pi\hbar$ being Planck's constant. Here

$$\sigma_j^x(t) = \mathrm{e}^{\mathrm{i}\mathcal{H}t/\hbar}\, \sigma_j^x\, \mathrm{e}^{-\mathrm{i}\mathcal{H}t/\hbar} \qquad (3.2)$$

is the (time-shifted) operator in the Heisenberg representation using the quantal Ising Hamiltonian

$$\mathcal{H} = -J \sum_{\langle l,k \rangle_0} \sigma_l^z \sigma_k^z - \theta J \sum_{\langle l,k \rangle_h} \sigma_l^z \sigma_k^z. \qquad (3.3)$$

As mentioned, the quantal form (3.3) is the classical form (2.1) wherein the Ising σ_l-variables have been replaced by their corresponding z-component Pauli spin operators σ_l^z.

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_N is defined as usual by the trace formula over all degrees of freedom of the system

$$Z_N = \operatorname*{Tr}_{\sigma} \mathrm{e}^{-\beta\mathcal{H}} \qquad (3.4)$$

whose inverse appears as the normalization factor in the expression for the canonical thermal average of any dynamical operator ξ:

$$\langle \xi \rangle = Z_N^{-1} \operatorname*{Tr}_{\sigma} \xi\, \mathrm{e}^{-\beta\mathcal{H}} \qquad (3.5)$$

where, in the last expressions (3.4) and (3.5), $\beta = 1/k_{\mathrm{B}}T$ with k_{B} being the Boltzmann constant and T the absolute temperature.

In order to evaluate the thermal average $\langle \sigma_n^x \sigma_m^x(t) \rangle$ in (3.1), one first introduces the following two useful identities:

$$g(\{\sigma_l^z\})\sigma_s^x = \sigma_s^x g(\{(-1)^{\delta_{ls}} \sigma_l^z\}) \qquad (3.6a)$$

$$\operatorname*{Tr}_{\sigma} \sigma_r^x \sigma_s^x g(\{\sigma_l^z\}) = \delta_{rs} \operatorname*{Tr}_{\sigma} g(\{\sigma_l^z\}) \qquad (3.6b)$$

where δ_{pq} is the usual Kronecker delta symbol and $g(\{\sigma_l^z\})$ is any function of the z-component Pauli spin operators σ of the total system. The proofs of both identities (3.6) are quite straightforward, namely, (3.6*a*) is proven by using elementary properties of the Pauli spin algebra and (3.6*b*) by conveniently choosing a direct product representation in which all σ_i^z-operators of the system are diagonal.

Using (3.2), (3.3), (3.5) and (3.6), one writes

$$
\begin{aligned}
\langle \sigma_n^x\ \sigma_m^x(t)\rangle &= Z_N^{-1} \operatorname*{Tr}_{\sigma} \sigma_n^x\, e^{i\mathcal{H}t/\hbar}\, \sigma_m^x\, e^{-i\mathcal{H}t/\hbar}\, e^{-\beta\mathcal{H}} \\
&= Z_N^{-1} \operatorname*{Tr}_{\sigma} \sigma_n^x \sigma_m^x \exp[(2it/\hbar) J\sigma_m^z(\sigma_{m_1}^z + \sigma_{m_2}^z + \theta\sigma_{m_3}^z)]\, e^{-\beta\mathcal{H}} \\
&= \delta_{nm}\langle \exp[(2it/\hbar) J\sigma_m^z(\sigma_{m_1}^z + \sigma_{m_2}^z + \theta\sigma_{m_3}^z)]\rangle \\
&= \delta_{nm}\langle \exp[i\omega_0 t\sigma_m^z(\sigma_{m_1}^z + \sigma_{m_2}^z + \theta\sigma_{m_3}^z)]\rangle
\end{aligned}
\tag{3.7}
$$

where m_1, m_2 and m_3 are the oblique and horizontal nearest-neighbouring sites of site m, respectively, and a characteristic circular frequency has been defined by $\omega_0 \equiv 2J/\hbar$. Substituting (3.7) into (3.1) gives

$$
\begin{aligned}
\mathcal{S}^{xx}(\boldsymbol{q}, \omega) &= \sum_n \frac{1}{2\pi}\int_{-\infty}^{\infty} dt \sum_m \exp[i\boldsymbol{q}\cdot(\boldsymbol{R}_m - \boldsymbol{R}_n) - i\omega t]\delta_{nm} \\
&\quad \times \langle \exp[i\omega_0 t\sigma_m^z(\sigma_{m_1}^z + \sigma_{m_2}^z + \theta\sigma_{m_3}^z)]\rangle \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega t} \sum_m \langle \exp[i\omega_0 t\sigma_m^z(\sigma_{m_1}^z + \sigma_{m_2}^z + \theta\sigma_{m_3}^z)]\rangle \\
&= \frac{N}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega t}\langle \exp[i\omega_0 t\sigma_0^z(\sigma_1^z + \sigma_2^z + \theta\sigma_3^z)]\rangle
\end{aligned}
\tag{3.8}
$$

where the numeric site labels 0, 1, 2, 3 in the final expression (3.8) are those previously specified in figure 1. Using (3.8), the *inelastic neutron scattering function*, $S^{xx}(\boldsymbol{q}, \omega)$, may now be written in the thermodynamic limit as

$$
S^{xx}(\boldsymbol{q}, \omega) \equiv \lim_{N\to\infty} N^{-1}\mathcal{S}^{xx}(\boldsymbol{q}, \omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega t}\langle \exp[i\omega_0 t\sigma_0(\sigma_1 + \sigma_2 + \theta\sigma_3)]\rangle
\tag{3.9}
$$

where, for notational simplicity in (3.9), the z-component Pauli spin operators have been replaced by the isomorphic Ising variables, and the thermal average within the integrand can now be associated with the infinite lattice (thermodynamic limit).

The exponential function appearing within the thermal average symbol in (3.9) is next expanded into a finite algebraic series by

$$
\begin{aligned}
\exp[i\omega_0 t(\sigma_0\sigma_1 + \sigma_0\sigma_2 + \theta\sigma_0\sigma_3)] &= A + B_1(\sigma_0\sigma_1 + \sigma_0\sigma_2) \\
&\quad + B_2\sigma_0\sigma_3 + C_1\sigma_1\sigma_2 + C_2(\sigma_1\sigma_3 + \sigma_2\sigma_3) + D\sigma_0\sigma_1\sigma_2\sigma_3
\end{aligned}
\tag{3.10}
$$

where

$$A = \tfrac{1}{8}[(f_3 + f_{-3}) + (f_2 + f_{-2}) + 2(f_1 + f_{-1})] \tag{3.11a}$$

$$B_1 = \tfrac{1}{8}[(f_3 - f_3) + (f_2 - f_{-2})] \tag{3.11b}$$

$$B_2 = \tfrac{1}{8}[(f_3 - f_{-3}) - (f_2 - f_{-2}) + 2(f_1 - f_{-1})] \tag{3.11c}$$

$$C_1 = \tfrac{1}{8}[(f_3 + f_{-3}) + (f_2 + f_{-2}) - 2(f_1 + f_{-1})] \tag{3.11d}$$

$$C_2 = \tfrac{1}{8}[(f_3 + f_{-3}) - (f_2 + f_{-2})] \tag{3.11e}$$

$$D = \tfrac{1}{8}[(f_3 - f_{-3}) - (f_2 - f_{-2}) - 2(f_1 - f_{-1})] \tag{3.11f}$$

where we have defined

$$f_{\pm 3} = e^{\pm i(2+\theta)\omega_0 t} \qquad f_{\pm 2} = e^{\pm i(2-\theta)\omega_0 t} \qquad f_{\pm 1} = e^{\pm i\theta\omega_0 t}. \tag{3.12}$$

To obtain the finite series expansion (3.10), use was made of the facts that each product of Ising variables is again an Ising variable, i.e. $\sigma_0\sigma_i = \pm 1$, $i = 1, 2, 3$, and thus satisfies $(\sigma_0\sigma_i)^{2m+1} = \sigma_0\sigma_i$, $(\sigma_0\sigma_i)^{2m} = 1$, $m = 0, 1, 2, \ldots$. The time-dependent coefficient expressions (3.11) were then determined by considering all possible realizations of the Ising σ-variables in the identity (3.10).

Substituting (3.10) into (3.9), one obtains

$$S^{xx}(q, \omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega t}(A + 2x_1 B_1 + x_1' B_2 + x_2 C_1 + 2x_2' C_2 + x_3 D) \tag{3.13}$$

where the equilibrium pair and quartet static correlations are defined by

$$\begin{aligned} &x_1 = \langle\sigma_0\sigma_1\rangle \qquad x_1' = \langle\sigma_0\sigma_3\rangle \qquad x_2 = \langle\sigma_1\sigma_2\rangle \\ &x_2' = \langle\sigma_1\sigma_3\rangle \qquad x_3 = \langle\sigma_0\sigma_1\sigma_2\sigma_3\rangle \end{aligned} \tag{3.14}$$

and the symmetry of the lattice has been recognized in the appropriate pairwise equating of geometrically equivalent pair correlations. As shown in the Appendix, all the above pair correlations x_1, x_1', x_2 and x_2' can be evaluated using complete elliptic integrals, and the four-spin correlation x_3 may then conveniently be evaluated in terms of x_2 and x_2' by means of a linear algebraic correlation identity. One notes, for the isotropic ($\theta = 1$) case, that the pair of nearest-neighbour correlations x_1, x_1' become degenerate as also do the pair of next-nearest-neighbour correlations x_2, x_2'.

Finally, substituting the coefficient expressions (3.11) and (3.12) into (3.13) and then utilizing the Fourier integral representation of the Dirac δ-function

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i(\omega-\eta)t} = \delta(\omega - \eta) \tag{3.15}$$

yields the result

$$S^{xx}(q, \omega) = \sum_n A_n \delta(\omega - \omega_n) \qquad n = \pm 3, \pm 2, \pm 1 \tag{3.16}$$

where the scattering amplitudes (intensities per site) are given as

$$A_{\pm 3} = \tfrac{1}{8}(1 \pm 2x_1 \pm x_1' + x_2 + 2x_2' \pm x_3) \tag{3.17a}$$

$$A_{\pm 2} = \tfrac{1}{8}(1 \pm 2x_1 \mp x_1' + x_2 - 2x_2' \mp x_3) \tag{3.17b}$$

$$A_{\pm 1} = \tfrac{1}{8}(2 \pm 2x_1' - 2x_2 \mp 2x_3) \tag{3.17c}$$

and the scattering frequencies by

$$\omega_{\pm 3} = \pm(2 + \theta)\omega_0 \qquad \omega_{\pm 2} = \pm(2 - \theta)\omega_0 \qquad \omega_{\pm 1} = \pm\theta\omega_0. \tag{3.18}$$

The elementary excitations of the present Ising model are, as usual, 'individual spin flips'. Expression (3.16) reveals that the inelastic neutron scattering only occurs at

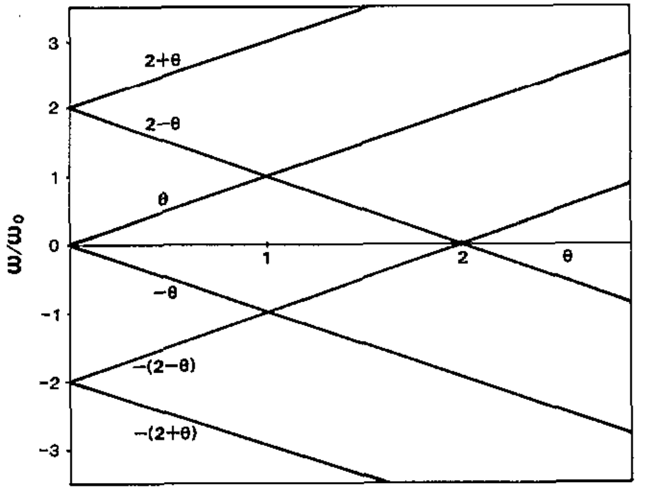

Figure 3. The (reduced) scattering frequencies ω/ω_0 versus the anisotropy parameter θ, where $\omega_0 \equiv 2J/\hbar$.

discrete energies where, for instance, $\hbar\omega_3 = (2+\theta)\omega_0$ is physically interpretable as the energy absorbed by the spin system upon 'flipping' a spin whose environmental spin configuration has the algebraic signatures ($\pm$) of the three nearest-neighbouring spins equal to the 'flipped' spin's original signature. As seen by (3.18), the discrete energy transfers $\hbar\omega_n(\theta)$, $n = \pm 3, \pm 2, \pm 1$, are independent of temperature, vary linearly with anisotropy θ and possess degeneracies. More specifically, one observes from (3.18) (see figure 3) that the pair of scattering frequencies ω_{+2}, ω_{+1} becomes essentially degenerate at $\theta = 1$ (isotropic case) as does the pair ω_{-2}, ω_{-1} while the pair ω_{+2}, ω_{-2} becomes accidentally degenerate at $\theta = 2$.

Since all the correlations appearing in the expressions (3.17) are exactly calculable as functions of temperature T and anisotropy θ (see the Appendix), the amplitudes (intensities per site) $A_n(T, \theta)$, $n = \pm 3, \pm 2, \pm 1$, of the Dirac δ-functions can be evaluated exactly and are displayed in figure 4 for all temperatures and selected values of the anisotropy. At very low temperatures, only the 'spin wave peak' at $\omega = \omega_3 = (2+\theta)\omega_0$ occurs, whereas the other peaks gain non-zero weight as the temperature is raised with the distribution of peaks becoming symmetric ($A_3 = A_{-3} = A_2 = A_{-2} = \frac{1}{8}$, $A_1 = A_{-1} = \frac{1}{4}$) at infinite temperature ($K = 0$). Since the honeycomb net is odd-coordinated (in fact, the only regular $d = 2$ lattice having an odd coordination number), there is no inelastic peak at $\omega = 0$ to combine with the elastic peak. Within the disordered regions ($T > T_c(\theta)$) of figure 4, the scattering intensities per site A_1, A_2 each exhibit a rounded maximum whose location and shape vary with the value of the anisotropy parameter θ (notice, for example, upon comparing figures 4(d) and 4(e), that the ordering in height of these two maxima reverses as θ becomes sufficiently small). Also, for fixed θ, the solution curves of $A_{\pm 3}$, $A_{\pm 2}$, $A_{\pm 1}$ provide evidence for finite-temperature *crossing points* whose locations vary with anisotropy. In figure 4, each of the six amplitudes $A_{\pm 3}$, $A_{\pm 2}$, $A_{\pm 1}$, has, for fixed θ, a weak *energy-type singularity* $\varepsilon \ln \varepsilon$ at the critical temperature $T_c(\theta)$ (see Figure 2) where $\varepsilon \equiv |T - T_c(\theta)|/T_c(\theta)$ is the fractional deviation of the temperature from its critical value. These $\varepsilon \ln \varepsilon$ branch point singularities are manifested as *vertical inflection points*, discernible on some of the curves in figure 4 with the chosen

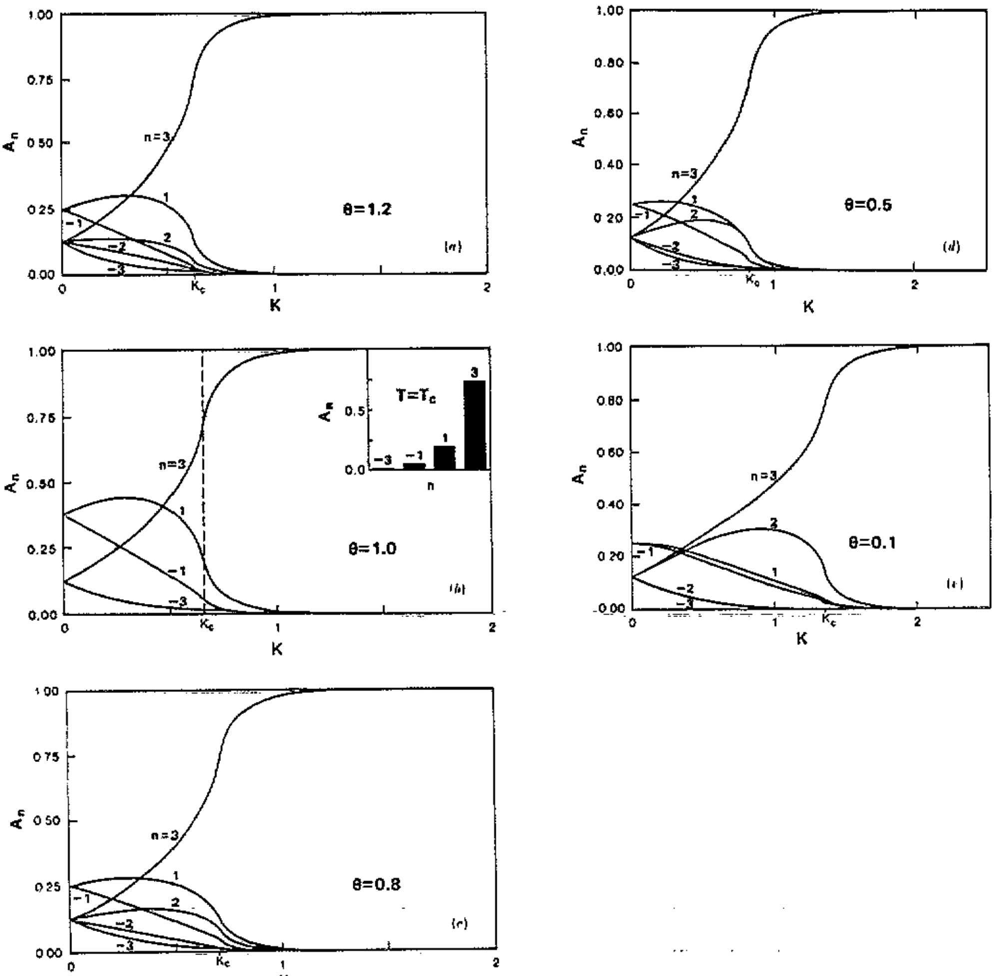

Figure 4. (*a*) Exact solution curves of the scattering amplitudes A_n versus the (dimensionless) interaction parameter K ($\equiv J/k_BT$) for the anisotropy parameter value $\theta = 1.2$. The critical value $K_c = 0.620\,04\ldots$. (*b*) Exact solution curves of the scattering amplitudes A_n versus the (dimensionless) interaction parameter K ($\equiv J/k_BT$) for the anisotropy parameter value $\theta = 1$ (isotropic case). Here, the amplitude notations A_1, A_{-1}, each embody a maximum threefold degeneracy in the discrete energy transfers. The inset graph shows the weights of the scattering amplitudes at criticality ($K = K_c \equiv J/k_BT_c = \frac{1}{2}\ln(2+\sqrt{3}) = 0.658\,47\ldots$). (*c*) Exact solution curves of the scattering amplitudes A_n versus the (dimensionless) interaction parameter K ($\equiv J/k_BT$) for the anisotropy parameter value $\theta = 0.8$. The critical value $K_c = 0.709\,73\ldots$. (*d*) Exact solution curves of the scattering amplitudes A_n versus the (dimensionless) interaction parameter K ($\equiv J/k_BT$) for the anisotropy parameter value $\theta = 0.5$. The critical value $K_c = 0.831\,44\ldots$. (*e*) Exact solution curves of the scattering amplitudes A_n versus the (dimensionless) interaction parameter K ($\equiv J/k_BT$) for the anisotropy parameter value $\theta = 0.1$. The critical value $K_c = 1.352\,25\ldots$.

scales (also note the differing restricted ranges of the scales). Furthermore, figure 5(*a*) displays the exact solution curves *at criticality* for the scattering amplitudes A_3, A_2, A_1 versus the anisotropy parameter θ, where it is observed that the amplitude A_3 possesses

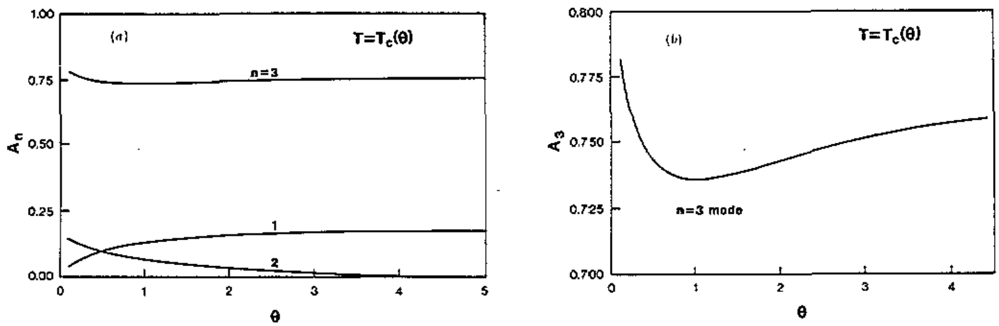

Figure 5. (*a*) Exact solution curves at criticality of the scattering amplitudes A_3, A_2, A_1 versus the anisotropy parameter θ. The curves for A_{-3}, A_{-2}, A_{-1} can be obtained from those shown by using detailed-balance relations. (*b*) Exact solution curve at criticality of the scattering amplitude A_3 versus the anisotropy parameter θ, focusing upon the minimal region.

a shallow asymmetric *minimum* at the value $\theta = 1$ (isotropic case) with figure 5(*b*) focusing upon this minimal region.

The scattering amplitudes (3.17) satisfy the sum rule $\Sigma_n A_n = 1$ confirming that the total integrated inelastic neutron scattering intensity per site, $\int_{-\infty}^{\infty} d\omega\, S^{xx}(q, \omega) = 1$, is independent of temperature and anisotropy which can likewise be proven by direct integration of the initial form (3.1). Also, it may be experimentally meaningful to remark that the linear algebraic relations (3.17) connecting the scattering amplitudes and localized Ising correlations are invertible, i.e. the *individual* pair and quartet static correlations can be determined in principle from precise experimental knowledge of *all* the scattering intensities.

Compared to the existence of only four inelastic scattering modes in the isotropic ($\theta = 1$) case, the present six modes illustrate the partial lifting of essential degeneracies. A more general anisotropic Ising Hamiltonian on the honeycomb lattice would contain two anisotropy parameters, say $\theta, \theta' > 0$, and would result in the complete lifting of the essential degeneracies, i.e. *eight* inelastic scattering modes appear. In this context, the facts that two of the four modes in the isotropic ($\theta = \theta' = 1$) case would each split into triplets can easily be established by an energy inspection upon an elementary 'star' cluster of Ising spins (a central spin and its three nearest-neighbouring spins). Veritably, such an energy inspection upon all possible configurations of the four-spin 'star' cluster gives the following eight scattering frequencies: $\pm(1 + \theta + \theta')\omega_0$, $\pm(1 + \theta - \theta')\omega_0$, $\pm(1 - \theta + \theta')\omega_0$, $\pm(1 - \theta - \theta')\omega_0$. For this more general case, since all localized even-number correlations appearing in the expressions for the inelastic scattering amplitudes possess weak (energy-type) singularities at the critical temperature $T_c(\theta, \theta')$ [6], each scattering amplitude therefore possesses this same nature of singularity at criticality. Moreover, these scattering intensities can be expected as previously to exhibit rounded extrema and crossing points.

4. Summary and conclusions

Exact results in physics are valuable for a variety of reasons. Endeavouring to retain only the most essential ingredients of a physical problem, exact solutions of simple model systems often provide definite guidance and insights on more realistic and therefore invariably more mathematically complex treatments. Also, exact results from tractable models of seemingly different physical systems may alert researchers to significant common features of these systems and actually emphasize concepts of universality. In addition to their aesthetic appeal, exact results can, of course, serve as standards against which both approximation methods and approximate results may be appraised.

In the present theoretical investigations, an exact solution has been calculated for the transverse dynamical spin correlation function $S^{xx}(q, \omega)$ of an anisotropic Ising model ferromagnet on the honeycomb lattice, having nearest-neighbour pairwise interactions J, $\theta J > 0$ along the oblique and horizontal lattice axes, respectively, with $\theta > 0$ being an anisotropy parameter. The form of this inelastic neutron scattering function was shown to be

$$S^{xx}(q, \omega) = \sum_{\substack{-3 \\ n \neq 0}}^{3} A_n(T, \theta)\delta(\omega - \omega_n(\theta))$$

which depends upon the frequency ω, temperature T and anisotropy θ. The discrete energy transfers $\hbar\omega_n(\theta)$ were independent of temperature, varied linearly with θ and possessed essential degeneracies at $\theta = 1$ (isotropic case) and an accidental degeneracy at $\theta = 2$. The amplitudes (intensities/site) $A_n(T, \theta)$ of the Dirac δ-functions exhibited, for fixed θ, such features as rounded maxima, crossing points, and weak (energy-type) singularities at the critical temperature $T_c(\theta)$. At criticality, the exact solution curve of the 'spin wave peak' scattering amplitude versus anisotropy gave evidence for a shallow asymmetric minimum at $\theta = 1$ (isotropic case). To our knowledge, the exact-solution continuous curves for the Ising scattering amplitudes at all temperatures and arbitrary values of the anisotropy are the first to be explicitly displayed in the literature, and as such were needed to reveal and examine the above features whose locations and shapes varied with anisotropy. When compared against the existence of only four inelastic scattering modes in the isotropic ($\theta = 1$) case, the present six modes illustrated the partial lifting of essential degeneracies. Some similar results were inferred for a more general case having two anisotropy parameters and eight modes.

The honeycomb lattice was chosen both for its small coordination number 3 which simplified the analyses and results, and for the fact that the exact solutions of all required Ising correlations could be obtained in a relatively straightforward manner in the presence of anisotropy. One can most probably expect, however, many of the same qualitative features appearing in the present results to arise similarly in the corresponding investigations upon the other three regular $d = 2$ lattices (square, kagomé and triangular). Further, for an alike Ising model in three dimensions ($d = 3$), the general form of the inelastic scattering function $S^{xx}(q, \omega)$ remains as previously, with each scattering amplitude again superposing a finite number of localized even-number correlations having energy-type singularities at the critical temperature. Consequently, one may speculate that the present $d = 2$ exact results could also provide insights and some qualitative interpretations for similar studies upon $d = 3$ regular lattices.

In real magnetic crystals, interactions extraneous to a strict Ising Hamiltonian, e.g. spin–lattice interactions, are essential to establish thermal equilibrium and to provide the noise for inciting thermal fluctuations. These additional perturbative interactions may influence the critical dynamics [7] of both the ordering (z-component) and non-ordering (x-, y-component) spin degrees of freedom, conceivably modifying critical features such as the weak singular behaviour $\varepsilon \ln \varepsilon$ of the transverse dyamical spin correlation function $S^{xx}(\boldsymbol{q}, \omega)$. Relevantly, in neutron scattering experiments, because of polarization factors in the cross-section, it is possible to separate or disentangle the dynamical spin correlation functions $S^{\alpha\alpha}(\boldsymbol{q}, \omega)$, $\alpha = x, y, z$. Indeed, elucidating the diverse complexities in dynamic critical phenomena is premised upon close collaborative contributions between theory and experiment.

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Appendix

As shown by Baxter and Enting [8], and Baxter [6], the honeycomb pair correlations x_1, x_1', x_2, x_2' needed in the present studies are related to the nearest-neighbour pair correlation of the anisotropic square Ising model.

More specifically, let $g_{sq}(K_h, K_v)$ be the horizontal nearest-neighbour pair correlation of a square lattice having (dimensionless) interaction coefficients K_h and K_v on the horizontal and vertical edges, respectively. Then

$$g_{sq}(K_h, K_v) = (\coth 2K_h) \int_0^{2K_h} \frac{a(l) - b(l) \tanh^2 x}{(1 + l^2 \sinh^2 x)^{1/2}} \, dx \tag{A1a}$$

where

$$l^{-1} = \sinh 2K_h \sinh 2K_v \qquad l_1 = 2l^{1/2}/(1+l)$$
$$a(l) = [(1+l)\,\mathrm{E}(l_1) + (1-l)\,\mathrm{I}(l_1)]/\pi \qquad b(l) = 2(1-l)\,\mathrm{I}(l_1)/\pi \tag{A1b}$$
$$\mathrm{I}(l_1) = \int_0^{\pi/2} dy\, (1 - l_1^2 \sin^2 y)^{-1/2} \qquad \mathrm{E}(l_1) = \int_0^{\pi/2} dy\, (1 - l_1^2 \sin^2 y)^{1/2}$$

with $\mathrm{I}(l_1)$, $\mathrm{E}(l_1)$ being, respectively, the complete elliptic integrals of the first and second kinds, of modulus l_1.

Using the relations derived by Baxter and Enting, one finds, upon letting

$$K' = \tfrac{1}{4}\ln\left(\frac{\cosh K(2+\theta)}{\cosh K(2-\theta)}\right) \tag{A2a}$$

$$K'' = \tfrac{1}{4}\ln\left(\frac{\cosh K(2+\theta)\cosh K(2-\theta)}{\cosh^2 K\theta}\right) \tag{A2b}$$

that

$$x_1 = g_{sq}(K, K') \quad x_2' = g_{sq}(K', K) \quad x_1' = g_{sq}(K\theta, K'') \quad x_2 = g_{sq}(K'', K\theta). \tag{A3}$$

Since the square lattice expression (A1*a*) is exactly calculable, equations (A3) now enable the honeycomb correlations x_1, x_1', x_2, x_2' to be exactly calculated.

By further employing a linear correlation identity whose coefficients depend only upon K and θ, the remaining quartet correlations x_3 can be found in terms of the next-nearest-neighbour pair correlations x_2 and x_2'. This may be seen as follows. Let $[g]$ be any function of the honeycomb Ising variables $\sigma_1, \sigma_2, \ldots, \sigma_{N-1}$ (*excluding* σ_0, the origin-site variable in figure 1). Using algebraic and partial-trace manipulations, one can derive the identity relation [9]

$$\langle \sigma_0[g] \rangle = \langle [g] \tanh K(\sigma_1 + \sigma_2 + \theta\sigma_3) \rangle \qquad \sigma_0 \notin [g]. \tag{A4}$$

Making use of fact that any dichotomic Ising variable σ_l satisfies $\sigma_l^{2n+1} = \sigma_l$, $\sigma_l^{2n} = 1$, $n = 0, 1, 2, \ldots$, the transcendental function of Ising variables appearing within the right-hand-side thermal average in (A4) can be expanded into a finite algebraic series as

$$\tanh K(\sigma_1 + \sigma_2 + \theta\sigma_3) = E_1(\sigma_1 + \sigma_2) + E_2\sigma_3 + F\sigma_1\sigma_2\sigma_3 \tag{A5}$$

where the coefficients E_1, E_2, F are determined by substituting all possible realizations of $\sigma_1, \sigma_2, \sigma_3$ into (A5), yielding

$$E_1 = \tfrac{1}{4}(\tanh K(2+\theta) + \tanh K(2-\theta)) \tag{A6a}$$

$$E_2 = \tfrac{1}{4}(\tanh K(2+\theta) - \tanh K(2-\theta) + 2\tanh K\theta) \tag{A6b}$$

$$F = \tfrac{1}{4}(\tanh K(2+\theta) - \tanh K(2-\theta) - 2\tanh K\theta). \tag{A6c}$$

Substituting (A5) into (A4) gives

$$\langle \sigma_0[g] \rangle = E_1\langle (\sigma_1 + \sigma_2)[g] \rangle + E_2\langle \sigma_3[g] \rangle + F\langle \sigma_1\sigma_2\sigma_3[g] \rangle \qquad \sigma_0 \notin [g] \tag{A7}$$

which is a *basic generating equation* for developing linear algebraic identities among multisite correlations of the anisotropic honeycomb Ising model (2.1) or its quantal version (3.3). For present purposes, an immediate application of (A7) yields

$$x_3 = \langle \sigma_0\sigma_1\sigma_2\sigma_3 \rangle = E_1\langle \sigma_2\sigma_3 + \sigma_1\sigma_3 \rangle + E_2\langle \sigma_1\sigma_2 \rangle + F = F + E_2x_2 + 2E_1x_2' \tag{A8}$$

where we have used the definitions (3.14), and the symmetry of the lattice has been recognized in the suitable pairwise equating of geometrically equivalent pair correlations. Since the exact solutions for x_2 and x_2' have already been determined, equations (A8) and (A6) now determine as desired the exact solution for the localized quartet correlation x_3.

Since Ising variables and z-component Pauli spin operators are isomorphic, these exact solutions for classical Ising correlations may be identified with the corresponding longitudinal Pauli spin correlations of the quantal Ising model (3.3) as needed.

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