# Neutron scattering solutions for an $S = 1/2$ quantum spin ladder

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## Abstract

A mapping of a two-dimensional $S = 1/2$ quantum spin ladder, having two-spin and four-spin interactions between spin sites, to a one-dimensional Ising chain enables the calculation of exact results for many physical quantities. Investigations into the ordering and spin states of the model develop a ground state phase diagram and provide possible insight into anomalous experimental results. A simulation of inelastic neutron scattering determines scattering intensities in the form of discrete amplitudes at absolute zero and finite temperatures.

## INTRODUCTION

Quantum spin ladders have been a subject of great interest to condensed matter researchers over recent years. Investigations of layered cuprate systems suggest that phenomena occurring in planes possessing ladder geometry may be the cause of high-$T_c$ superconductivity in the material [1]. Another exciting application in the study of spin ladders arises from the fact that the structures show evidence of quantum critical phase transitions, namely transitions taking place at absolute zero as opposed to thermal phase transitions at finite temperatures.

Most modeling of these intriguing systems has been based on interactions between pairs of sites on the ladder structure. One proposed model makes use of two-spin interactions (between two spin-1/2 sites on the same rung) and four-spin interactions (between four sites on two rungs). In mapping the Hamiltonian of this two-dimensional ladder system to a one-dimensional Ising chain model, exact solutions for correlations between ladder sites become attainable, in turn leading to projected results for neutron scattering.

Since neutrons are spin-1/2 and chargeless they make for an ideal medium of scattering to analyze the spectral properties of this ladder model. The correlations between ladder sites allow the scattering function (an extremely important part of the scattering cross-section for inelastic neutron scattering) to be solved. This function reduces to seven discrete intensities of neutrons scattered from the ladder as a function of temperature, energy transfer, and values of interaction parameters. Computational analysis of these results yields essential information on the energy levels and spin states of the ladder model. The wealth of knowledge gleaned from the scattering simulation can also further characterize real ladder materials currently being tested.

## $S = 1/2$ SPIN LADDER MODEL

The proposed model consists of $N$ sites along a two-legged ladder (having $N_r = N/2$ rungs), each with $S = 1/2$ spin. In the interests of attaining exact solutions, periodicity is imposed on the ladder by attaching the sites labeled $N$ and $N - 1$ to the sites labeled one and two (see Figure 1). A two-spin interaction along the rungs and a four-spin interaction

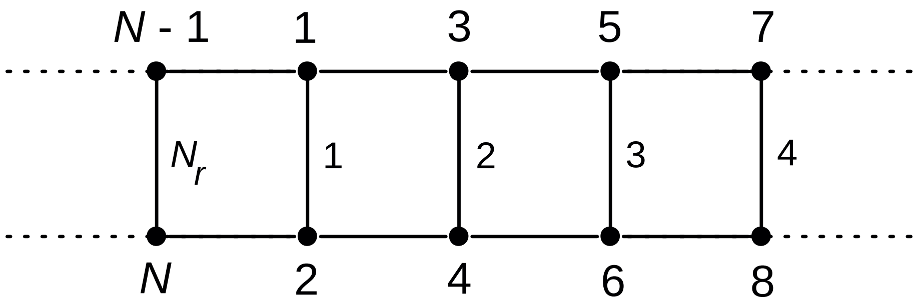


FIG. 1: The two-legged quantum spin ladder has $N$, $S = 1/2$ spin sites with imposed periodicity.

between the sites on two rungs define the Hamiltonian of the system as

$$\mathcal{H} = -\sum_{j=1}^{N_r} \left[ J_2\, \boldsymbol{\sigma}_{2j-1} \cdot \boldsymbol{\sigma}_{2j} + J_4 (\boldsymbol{\sigma}_{2j-1} \cdot \boldsymbol{\sigma}_{2j})(\boldsymbol{\sigma}_{2j+1} \cdot \boldsymbol{\sigma}_{2j+2}) + \mu h^z (\sigma^z_{2j-1} + \sigma^z_{2j}) \right] \quad , \tag{1}$$

where $\boldsymbol{\sigma}_i = 2\boldsymbol{S}_i/\hbar$ for sites $i = 1, 2, \ldots, N$ are Pauli spin operators, $J_2$ and $J_4$ are parameters of the two-spin and four-spin Heisenberg interactions, respectively. A longitudinal magnetic field $\mu h^z$, with $\mu$ as the electron intrinsic magnetic moment, interacts with the $z$ components of the spins.

A previous article on this model by Barry and Meisel employed a rung transfer matrix method (in which energy eigenvalues of the Hamiltonian operating on adjacent rungs are arranged according to spin states) to solve for the partition function $Z = \text{Trace}\, e^{-\beta\mathcal{H}}$, with $\beta = 1/kT$ (where $k$ is the Boltzmann constant and $T$ is temperature) [2]. Knowledge of $Z$ allowed many thermodynamic quantities of the system to be determined, such as free energy and entropy per rung. These properties enabled development of a picture of the ground state ($T = 0$) of the system for varying values of the interaction parameters $J_2$ and $J_4$ (see Figure 2). Interestingly, at $T = 0$ and $h^z = 0$, the spin states of the rungs of the ladder do not depend explicitly on the values of the interaction parameters themselves but rather their ratio ($\alpha = J_2/J_4$). For ray lines in $J_2 - J_4$ space between $\alpha = 2$ in the first quadrant and $\alpha = 6$ in the third quadrant, the two $S = 1/2$ spins on the rungs of the ladder combine as singlets. Between $\alpha = 2$ in the first quadrant and $\alpha = -2$ in the second quadrant, the rungs have a triplet ground state, and from $\alpha = -2$ in the second quadrant and 6 in the third quadrant, the rungs alternate between singlets and triplets, giving rise to a "staggered region" in $J_2 - J_4$ space.

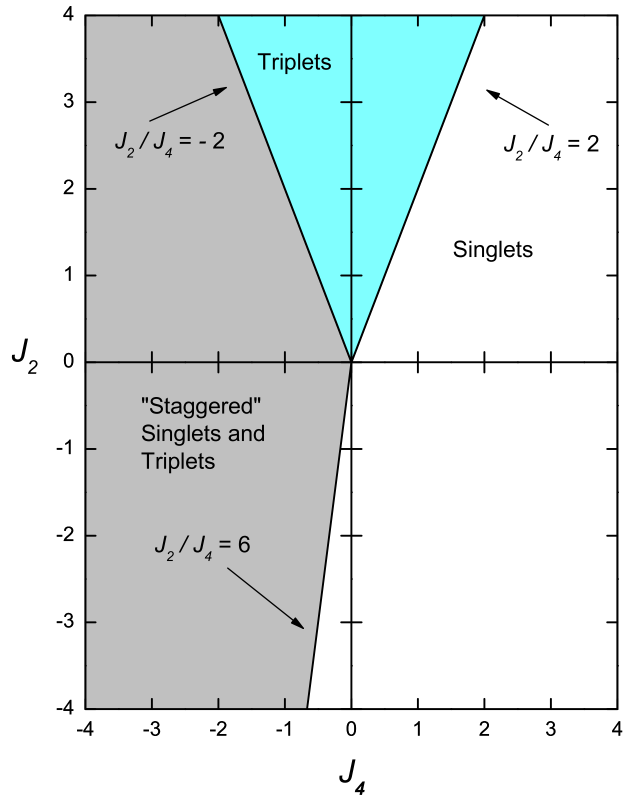


FIG. 2: The $T = 0$ phase diagram in $J_2 - J_4$ interaction parameter space has boundaries at $\alpha = 2$ (first quadrant) separating the singlet state (white) and the triplet state (blue shaded); at $\alpha = -2$ (second quadrant) between the triplet state and the "staggered" state of alternating singlets and triplets (gray shaded); and at $\alpha = 6$ (third quadrant) between the "staggered" region and the singlet region.

Since the rung orientations in Figure 2 occur in the ground state of the model, the ray lines $\alpha = -2$, 2, and 6 serve as quantum phase boundaries (as opposed to thermal phase boundaries occurring at finite temperatures). Quantum critical transitions have captured intense interest in recent years with collapsing energy scales and rapid changes in the orderings of systems [3]. These phenomena manifest themselves in diverging length scales and discontinuous behavior in physical properties that emerge from the exact results discussed in later sections of this paper.

## ISING CHAIN REPRESENTATION OF THE MODEL

Taking advantage of the rung symmetry of the ladder model, one can replace the single site spin operators $\sigma_i$ with rung spin operators by

$$\mu_j \equiv \frac{1}{2}(\boldsymbol{\sigma}_{2j-1} \cdot \boldsymbol{\sigma}_{2j} + 1) \quad , \tag{2}$$

with the scale factors chosen such that

$$\mu_j = \begin{cases} +1 & \text{triplet states of } j^{\underline{th}} \text{ rung,} \\ -1 & \text{singlet state of } j^{\underline{th}} \text{ rung.} \end{cases} \tag{3}$$

This change of variables results in the partition function taking the form of that of an Ising chain, an extensively studied model with many exact results in the literature [4]. With Ising variables, the Hamiltonian of the ladder model becomes

$$\mathcal{H}^* = -\left[ J_2^* \sum_{\langle i,j \rangle} \mu_i \mu_j + \mu h^{z*} \sum_j \mu_j \right] \quad , \tag{4}$$

where $J_2^* = 4J_4$ denotes a pair interaction between neighboring sites on the chain equivalent to the four spin interaction on the ladder. The transformation also produces a magnetic field along the chain $\mu h^{z*} = 2(J_2 - 2J_4) + \frac{1}{2\beta} \ln(2\cosh 2\beta\mu h^z + 1)$, which has an effective temperature dependence ($\beta = 1/kT$) arising from the temperature dependence of the spin states of the rungs.

Reducing the dimensions of the problem from the two-dimensional ladder to the one-dimensional chain simplifies calculations of correlations between spin sites (namely in diagonalizing matrices of rank 2 instead of rank 4). Well established results applied to the present model's partition function produce

$$\langle \mu_j \rangle = (\sinh \mu h^{z*})(\sinh^2 \mu h^{z*} + e^{-4\beta J_2^*})^{-1/2} \quad , \tag{5}$$

$$\langle \mu_i \mu_j \rangle = \langle \mu_i \rangle^2 + (1 + e^{4\beta J_2^*} \sinh^2 \mu h^{z*})^{-1} (\lambda_-/\lambda_+)^{j-i} \quad , \qquad j \geq i, \tag{6}$$

with $\lambda_\pm$ emerging as eigenvalues from the Ising chain transfer matrix. The $\langle \ldots \rangle$ notation signifies a thermal average of quantum mechanical operators, the computation of which features prominently in the neutron scattering theory developed by van Hove, from which the simulated scattering in this paper takes its form [5].

From Eq. 2, one can now relabel ladder rung sites as Ising chain sites,

$$\mu_1 = \frac{\boldsymbol{\sigma}_2 \cdot \boldsymbol{\sigma}_2 + 1}{2}, \qquad \mu_0 = \frac{\boldsymbol{\sigma}_3 \cdot \boldsymbol{\sigma}_4 + 1}{2}, \qquad \text{and} \qquad \mu_2 = \frac{\boldsymbol{\sigma}_5 \cdot \boldsymbol{\sigma}_6 + 1}{2}. \tag{7}$$

Relationships between Ising variables now organize as $\langle\mu_0\rangle$ defined as a local magnetization, $\langle\mu_0\mu_1\rangle$ representing the first neighbor pair correlation (between two sites on the chain separated by one rung spacing), $\langle\mu_1\mu_2\rangle$ representing the second neighbor pair correlation (between two sites separated by two rung spacings), and continure in this fashion for thermal averages of any number of Ising variables.

The presence of $\lambda_-/\lambda_+$ to powers of inter-rung spacings in correlation functions suggests a characteristic length scale $\eta$ for the model, which arises as

$$\eta = (\ln|\lambda_+/\lambda_-|)^{-1} \quad , \tag{8}$$

with dimensions of inter-rung spacings. The magnitude of $\eta$ gives a measure of the ordering of the system as the number of lattice distances over which two spins correlate with one another. Figures 3a and 3b exhibit the thermal evolution of $\eta$ for ratios $\gamma = J_4/J_2$ in all quadrants of $J_2 - J_4$ space. In the singlet and triplet regions of the phase diagram (Fig. 2), the magnitude of $\eta$ goes to zero as $T$ approaches zero and infinity, and in the singlet region has a peak at finite temperatures. The sharp peak in correlation length in the first quadrant of $J_2 - J_4$ space (Fig. 3a) reaches on order of $10^6$, suggesting short to intermediate range ordering in the system, while the rounded maximum in the fourth quadrant (Fig. 3b) indicates only short range ordering. In the "staggered" region of $J_2 - J_4$ space, $\eta$ approaches infinity as $T$ goes to zero. This diverging length scale evinces a quantum critical ground state and long range ordering for the "staggered" region. Finally on the phase boundary lines $\alpha = -2$, 2, and 6, $\eta$ stays finite at $T = 0$.

## NEUTRON SCATTERING SIMULATION

In any scattering experiment, the double differential scattering cross section (the fraction of neutrons scattered between angles $\Omega$ and $\Omega + d\Omega$ with an energy between $E$ and $E + dE$ [6]) must be solved. For neutron scattering [5],

$$\frac{d^2\sigma}{d\Omega dE} = (\frac{\gamma' e^2}{mc^2})^2 \, \frac{N_s}{\hbar} \, \frac{k_1}{k_0} \, |F(\boldsymbol{q})|^2 \sum_{ij} (\delta_{ij} - \cos q_i \cos q_j) \mathcal{S}^{ij}(\boldsymbol{q}, \omega) \quad . \tag{9}$$

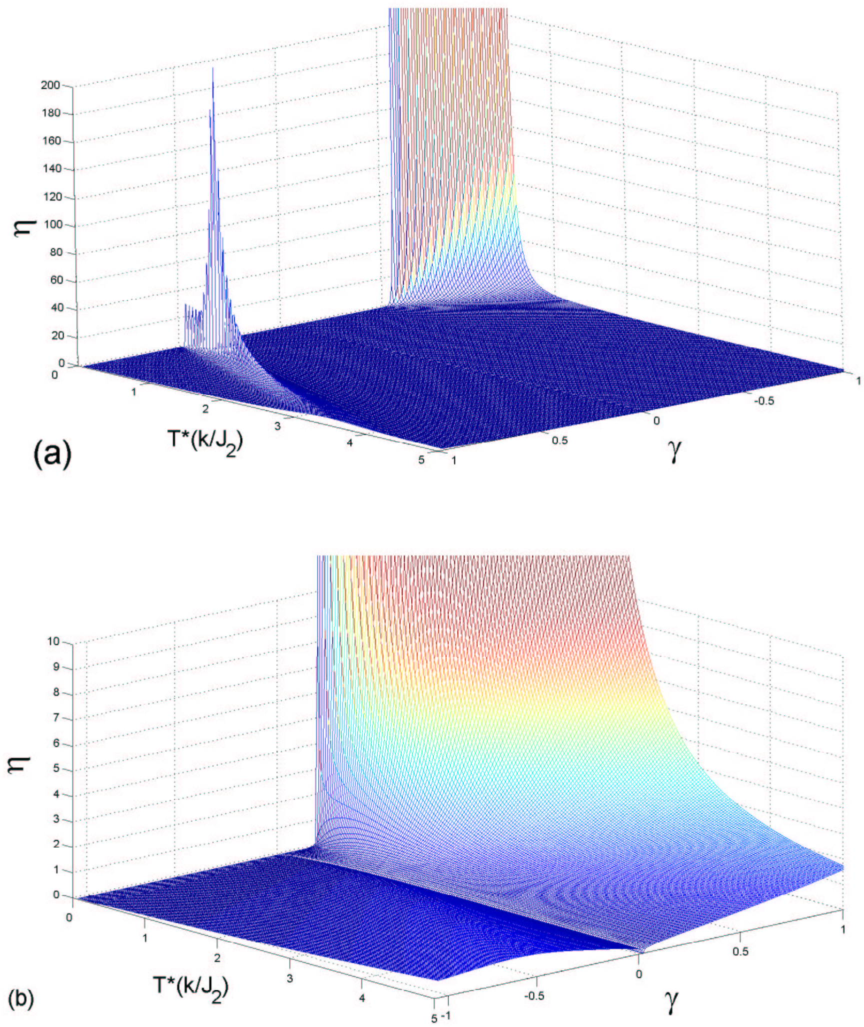


FIG. 3: Correlation length $\eta$ as a function of reduced temperature $T(k/J_2)$ and $\gamma = J_4/J_2$ shows drastically different behavior for different quadrants of $J_2 - J_4$ space. (a) The singlet region features local maxima at finite temperatures, and along with the triplet region, $\eta$ goes to zero in the ground state. (b) Correlation length in the "staggered" region goes to infinity at $T = 0$, exhibiting long range ordering.

Here $e$ and $m$ are the electron charge and mass, $N_s$ is the number of scattered neutrons, $\gamma'$ is the neutron magnetic moment, $\boldsymbol{k}_0$ and $\boldsymbol{k}_1$ are the initial and final wave vectors of the neutrons, $\boldsymbol{q} = \boldsymbol{k}_0 - \boldsymbol{k}_1$, $\hbar\omega$ is the energy transfer of the neutrons, and $F(\boldsymbol{q})$ is a form factor given by the spin structure of the target sample. The scattering or response function $\mathcal{S}^{ij}(\boldsymbol{q}, \omega)$ is evaluated over different coordinate indices in the sum $\sum_{ij}$. For the Ising model, only the $x$ and $y$ components of the scattering function contribute to inelastic scattering, and $\mathcal{S}^{yy}(\boldsymbol{q},\omega) = \mathcal{S}^{\,xx}(\boldsymbol{q},\omega)$. Thus solving for $\mathcal{S}^{\,xx}(\boldsymbol{q},\omega)$ determines the entire neutron scattering response function;

$$\mathcal{S}^{\,xx}(\boldsymbol{q},\omega) = \sum_n \frac{1}{2\pi}\int_{-\infty}^{\infty} dt \sum_m \exp[i\boldsymbol{q}\cdot(\boldsymbol{R}_m - \boldsymbol{R}_n) - i\omega t]\langle\sigma_n^x\sigma_m^x(t)\rangle \quad , \tag{10}$$

with $R_m$ and $R_n$ being position vectors for sites $m$ and $n$ on the ladder.

Through symmetry considerations, the only non-zero contributions to $\mathcal{S}^{\,xx}(\boldsymbol{q},\omega)$ come from $q = 0$ and $q = \pi/a$, where $a$ is the distance between two adjacent rungs. Substitutions of Ising variables for ladder variables (Equation 7) unfold Eq. 10 as

$$\mathcal{S}^{\,xx}(0,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega\, t}\langle\frac{2}{3}(\mu_0+1)\, e^{i\tilde{\omega}_{\mu_0,\mu_1,\mu_2}\, t}\rangle, \tag{11a}$$

$$\mathcal{S}^{\,xx}(\frac{\pi}{a},\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega\, t}\langle\frac{2}{3}(2-\mu_0)\, e^{i\omega_{\mu_0,\mu_1,\mu_2}\, t}\rangle. \tag{11b}$$

where the labels $\mu_0$, $\mu_1$, and $\mu_2$ can take values of plus or minus, and the temperature-independent scattering frequencies are defined as

$$\omega_3 \equiv \omega_{+++} = -\omega_{-++} = 4\hbar^{-1}(J_2 + 2J_4), \tag{12a}$$

$$\omega_1 \equiv \omega_{++-} = \omega_{+-+} = -\omega_{-+-} = -\omega_{--+} = 4\hbar^{-1}(J_2 - 2J_4), \tag{12b}$$

$$\omega_2 \equiv \omega_{+--} = -\omega_{---} = 4\hbar^{-1}(J_2 - 6J_4), \tag{12c}$$

and

$$\omega_{-3} \equiv \tilde{\omega}_{-++}/2 = -4\hbar^{-1}(J_2 + 2J_4) = -\omega_3, \tag{13a}$$

$$\omega_{-1} \equiv \tilde{\omega}_{-+-}/2 = \tilde{\omega}_{--+}/2 = -4\hbar^{-1}(J_2 - 2J_4) = -\omega_1, \tag{13b}$$

$$\omega_{-2} \equiv \tilde{\omega}_{---}/2 = -4\hbar^{-1}(J_2 - 6J_4) = -\omega_2. \tag{13c}$$

Since the function $\mathcal{S}^{\,xx}(\boldsymbol{q},\omega)$ now spans over discrete variables $q$ and $\omega$, the integral in Eqs. 11a and 11b turns into a sum over distinct states,

$$\mathcal{S}^{xx}(0,\omega) = A_0\delta(\omega) \quad , \tag{14a}$$

$$\mathcal{S}^{xx}(\frac{\pi}{a},\omega) = \sum_n A_n\delta(\omega - \omega_n) \quad , \qquad n = \pm 3, \pm 2, \pm 1, \tag{14b}$$

and $A_n$ give temperature-dependent scattering amplitudes with physical significance as intensity of neutron scattering per ladder site. The amplitudes corresponding to the previously defined scattering frequencies depend on the correlations along the Ising chain as

$$A_3 = \frac{1}{12}(1 + 3\langle\mu_0\rangle + 2\langle\mu_0\mu_1\rangle + \langle\mu_1\mu_2\rangle + \langle\mu_0\mu_1\mu_2\rangle) \tag{15a}$$

$$A_{-3} = \frac{1}{4}(1 + \langle\mu_0\rangle - 2\langle\mu_0\mu_1\rangle + \langle\mu_1\mu_2\rangle - \langle\mu_0\mu_1\mu_2\rangle) \tag{15b}$$

$$A_2 = \frac{1}{12}(1 - \langle\mu_0\rangle - 2\langle\mu_0\mu_1\rangle + \langle\mu_1\mu_2\rangle + \langle\mu_0\mu_1\mu_2\rangle) \tag{15c}$$

$$A_{-2} = \frac{1}{4}(1 - 3\langle\mu_0\rangle + 2\langle\mu_0\mu_1\rangle + \langle\mu_1\mu_2\rangle - \langle\mu_0\mu_1\mu_2\rangle) \tag{15d}$$

$$A_1 = \frac{1}{6}(1 + \langle\mu_0\rangle - \langle\mu_1\mu_2\rangle - \langle\mu_0\mu_1\mu_2\rangle), \tag{15e}$$

$$A_{-1} = \frac{1}{2}(1 - \langle\mu_0\rangle - \langle\mu_1\mu_2\rangle + \langle\mu_0\mu_1\mu_2\rangle), \tag{15f}$$

$$A_0 = \frac{2}{3}(1 + \langle\mu_0\rangle), \tag{15g}$$

where

$$\langle\mu_0\,\mu_1\,\mu_2\rangle \;=\; \mathcal{A}\,\langle\mu_1\,\mu_2\rangle \;+\; 2\,\mathcal{B}\,\langle\mu_1\rangle \;+\; \mathcal{C} \tag{16}$$

enters as a linear combination of local magnetization $\langle\mu_1\rangle$ and second neighbor pair correlation $\langle\mu_1\mu_2\rangle$, with coefficients arising out of the partition function operating on Ising variables.

## RESULTS AND DISCUSSION

Figures 4 and 5 demonstrate the drastic qualitative differences between the scattering amplitudes and correlations from which they arise for ray lines in the first and third quadrants of $J_2 - J_4$ space. The prevalence of $A_{-2}$ in the ground state of the first quadrant (Fig. 4b) speaks to the presence of a finite energy transfer at $T = 0$, a feature which does not appear in the more diverse spectrum in the third quadrant (Fig. 5b). Another intriguing characteristic emerges in the observation that the spatial correlations in the third quadrant (Fig. 5a) saturate to infinite temperature limits at higher temperatures that those in the first quadrant (Fig. 4a). This property suggests that some interesting physics can be studied at relatively high temperatures for ladder systems with $J_2$ and $J_4 < 0$ (corresponding to antiferromagnetic interactions).

While the proposed model may not exactly match any actual materials, the exact solutions gained from keeping the model simple can yield great insight and direction into future studies of ladder systems. The complete excitation spectrum of a ladder with two-spin and four-spin interactions has been calculated as a function of temperature, energy and interaction parameters. The explorations into the ordering of such a system can provide new outlooks on the origin of high-$T_c$ superconductivity in ladder systems. Evidence of quantum critical phase transitions have revealed themselves, further developing another topic of great research interest.

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**REFERENCES**

[1] K. P. Schmidt and G. S. Uhrig, Mod. Phys. Lett. B **19**, 1179 (2005).

[2] J. H. Barry and M. W. Meisel, Phys. Rev. B **58**, 3129 (1998).

[3] A. J. Schofield, Science **315**, 945 (2007).

[4] G. A. T. Allan and D. D. Betts, Can. J. Phys. **46**, 799 (1967).

[5] L. Van Hove, Phys. Rev. **95**, 249, 1374 (1954).

[6] S. W. Lovesey, *Theory of Neutron Scattering from Condensed Matter* (Oxford, Clarendon, 1984).

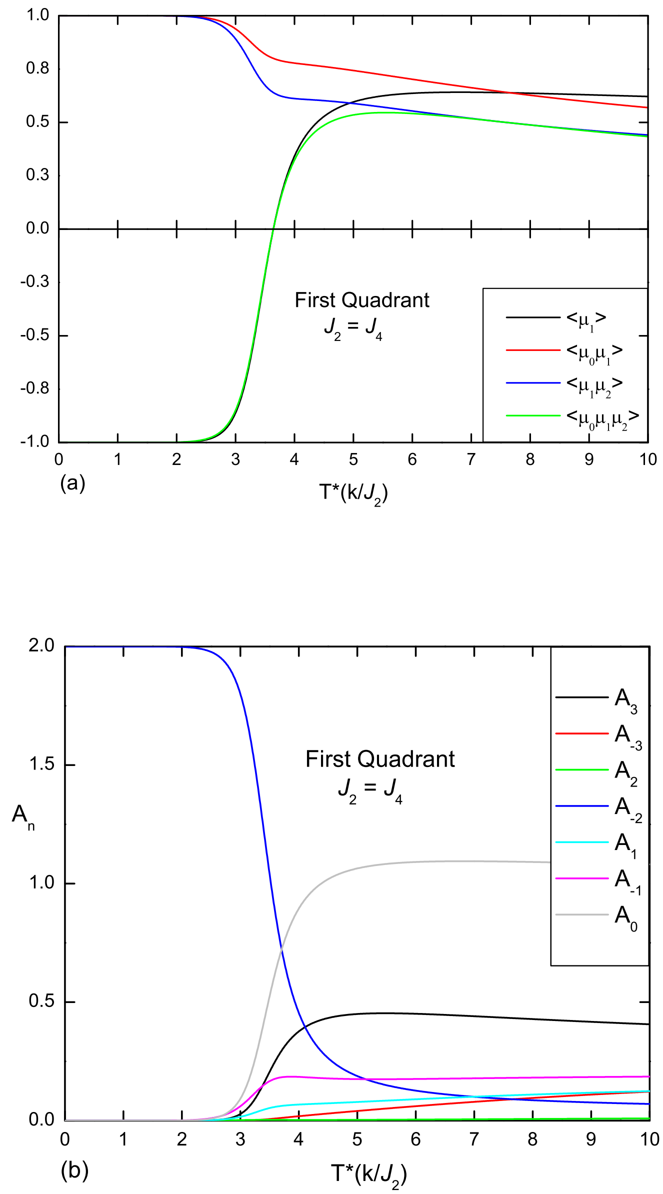
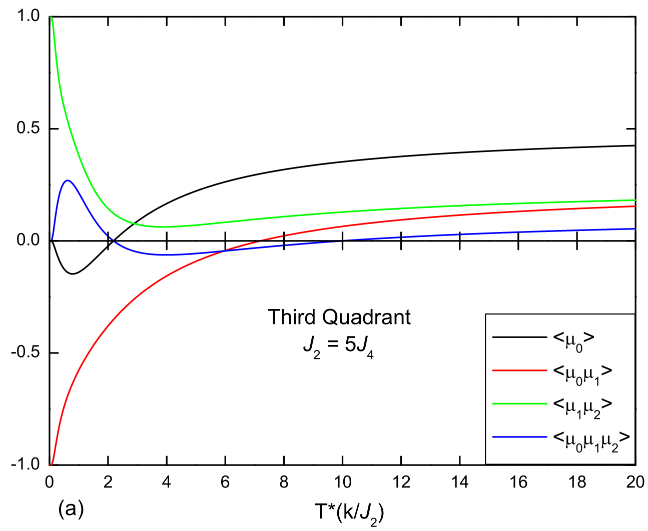



FIG. 4: (a) Ising correlations and (b) neutron scattering amplitudes for the specific ray line $J_2 = J_4$ in the first quadrant of $J_2 - J_4$ space. On this ray line, as well as all others in the singlet region, the dominance of $A_{-2}$ in the ground state produces a positive, $T = 0$ energy transfer.



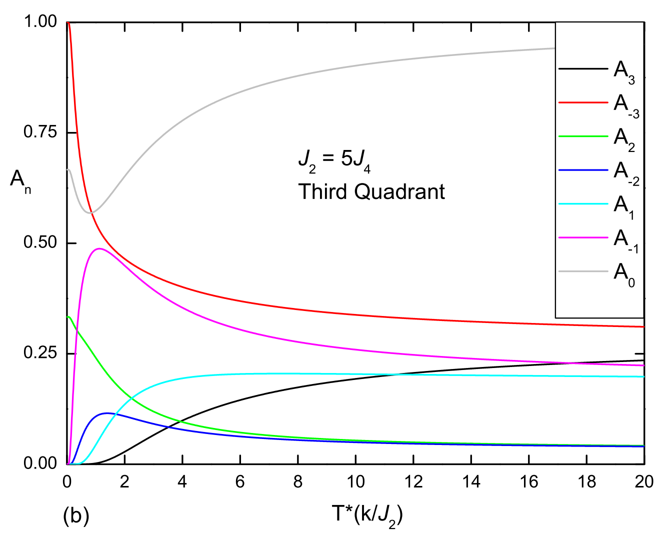




FIG. 5: (a) Ising correlations and (b) neutron scattering amplitudes in the third quadrant of $J_2 - J_4$ space for the ray line $J_2 = 5J_4$. This ray line features a qualitatively different ground state from the first quadrant (Fig. 4); the odd numbered Ising correlations ($\langle\mu_0\rangle$ and $\langle\mu_0\mu_1\mu_2\rangle$) go to zero whereas in the first quadrant they go to 1 at ($T = 0$), and the even numbered correlations $\langle\mu_0\mu_1\rangle$ and $\langle\mu_1\mu_2\rangle$ alternate in sign as opposed to the degeneracy in the first quadrant. The ground state also features diverse amplitudes, the energy transfer of which collectively add to zero, in contrast to the ground state energy transfer in the first quadrant.