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Quantum Spin Chains

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Introduction

Serious scientific interest in one-dimensional (1-D) physics arose in the early 1960's. This interest was stimulated by exact as well as accurate numerical solutions to a variety of quantum spin chain problems [1]. The potential relevance of such solutions to real experimental systems was first demonstrated by Griffiths [2] in conjunction with workers at the Kamerlingh Onnes Laboratorium, Leiden. Theory and experiment were shown to be in excellent agreement for a naturally quasi-1-D Heisenberg spin 1/2 antiferromagnet, copper tetrammine sulphate $[Cu(NH_3)_4SO_4 \cdot H_2O]$. Further stimulus to the new field of quasi-1-D magnetism was provided by an annotated collection of reprinted papers on a variety of 1-D model systems, including lattice gases, dynamical disordered crystal lattices, many-fermion gases (electron gases) as well as magnets. The collection appeared in book form, and remains today an important introduction to 1-D theory [3].

Interest in quantum spin chains has developed in surges. Initial enthusiasts were primarily experimental physicists who attempted to identify naturally occurring quasi-1-D magnetic insulators or who performed 'magnetic engineering' by substituting large non-magnetic organic 'spacer' molecular complexes like pyridines or pyrazines in place of, say, water molecules. The chains of magnetic ions were thus forced further apart and the 1-D characteristics of the substance much enhanced. The goal was to provide experimental realizations of a variety of spin chain models. As the zoo of experimental animals neared completion, interest among physicists started to wane, but compensation was provided by growing interest among coordination chemists. Since the theory of superexchange remains on a far from secure footing, chemists are tending to investigate empirically the variation of exchange constant with bond length and bond angle (and possibly other factors like ligand orientation). They make use of homologous families of 1-D magnets, relying on the complete and accurate statistical mechanical knowledge not available in higher-D systems. One important source of uncertainty in the processing of the data is thus removed.

In the early 1970's a new class of naturally anisotropic, quasi-1-D systems came into vogue. These are organic conductors, semi-conductors, and even insulators [4]. Materials like the famous TTF-TCNQ are called organic metals because of their high conductivity at low temperature with its negative temperature coefficient. Considerable excitement and also some controversy was generated by a prediction by Little [5] that organic conductors might show 'high temperature' superconductivity at, say, 50 K. Despite several years of intense effort, the Little prediction has not come close to being realised. However, research is continuing with renewed stimulation by the recent discovery of a new member of the class, which goes superconducting at 12 kbar pressure with a transition at 0.9 K [6]. What interests us here is that even the conducting members of this large class of quasi-1-D organics can be described by 1-D models directly related to quantum spin chains.

It appears, however, that currently the greatest interest in quantum spin chains arises from their intimate relation to non-trivial lattice gauge field theories having one space and one time dimension. The relevant field theory solutions or excitations commonly have soliton character and are of high interest to particle physicists.

Several reviews of the state of the art in 1-D physics have appeared rather recently. Early analytical work beginning in the 1930's has been reviewed by THOMPSON [7] and more recent theoretical developments by BONNER [1], and theory with emphasis on spin dynamics by STEINER, VILLAIN and WINDSOR [8] and BIRGENEAU and SHIRANE [9]. Other reviews with strong emphasis on dynamics include articles by RICHARDS [10] and HONE and RICHARDS [11]. A series of reviews by DE JONGH features quasi-1-D theory and experiment [12]. Quasi-1-D experimental systems from the viewpoint of a chemist are reviewed by CARLIN [13]. Finally, a recent article by KOGUT [14J] gives a clear and detailed discussion of the relation of quantum spin chains and related models to lattice field theories.

The focus of this paper will be several very recent developments in the theory of spin chains, including both static and dynamical properties. Random 1-D systems are not considered. The striking feature of recent work of non-random systems has been the importance of quantum effects, and classical models will be discussed only in relation to differences in behavior between them and their quantum counterparts. Specifically, we shall concentrate on (i) the current analytic status of spin chains, (ii) 1-D models exactly solvable by the famous Bethe Ansatz and also mappings between models which give several solutions for the price of one, (iii) the current status of numerical studies on spin chains, (iv) alternating (dimerized) chains, relevant to organic conductors and insulators, (v) a new quantum renormalization group method, and (vi) a novel approach to quantum spin dynamics.

Spin Chains: Current Analytic Status

The effective spin Hamiltonian for the general quantum spin chain may be written:

$$\mathcal{H} = -2J \sum_{i=1}^{N} \left\{ a s_i^z s_{i+1}^z + b s_i^x s_{i+1}^x + c s_i^y s_{i+1}^y \right\}. \tag{1}$$

We have bilinear spin coupling, assume nearest-neighbor spin interactions only, and the effective exchange constant is J, modified for the spin couplings in different directions by factors a, b and c. The *Ising model* is obtained by putting $b = c = 0$ (in general, by letting any two of a, b, c equal zero). The *XY model* is obtained by putting $a = 0$ (in general by letting any one of a, b, c equal zero). If $a = b = c$, we have complete rotational symmetry in spin space and obtain the *Heisenberg model* which may, of course, be written in vector form

$$\mathcal{H} = -2J \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1}. \tag{2}$$

If $J > 0$, the spins may lower their energy by aligning parallel and we have a Heisenberg ferromagnet. If $J < 0$, the antiparallel spin arrangement is favored and we have an antiferromagnet. If a, b and c are not equal we have spin anisotropy. If $a > b \simeq c$, we have uniaxial (easy axis) anisotropy. On the other hand, if $a < b \simeq c$, easy plane anisotropy results. The effects of an applied magnetic field can be represented by the addition of a general Zeeman term $-g\beta\vec{H} \cdot \sum \vec{S}_i$ to Hamiltonian (1). Finally, the spin value may range over $1/2 \leq S \leq \infty$.

The static properties commonly measured by experimentalists are the initial (zero field) susceptibility χ, the specific heat at constant field C_H, and the magnetization isotherms as a function of

applied field, M_T vs H. In dynamics the Fourier transforms of the spin-spin correlation functlons are important. The 1-D spin-1/2 Ising model was first solved in 1925 (ISING [15]). A complete description including correlation function properties may be found in THOMPSON [7]. The 1-D spin-1/2 XY model was solved analytically in the early 1960's, independently by LIEB, SCHULTZ and MATTIS [16] with emphasis on correlation functions (see also later work by PFEUTY[17]), and by KATSURA [18] with emphasis on the thermal and magnetic properties. KATSURA [18] and PFEUTY [17] also obtained exact results for the transverse Ising model. This interesting model results from taking $b = c = 0$ in (1) and retaining, say, only the X component of the Zeeman term. Since spin-spin interaction and applied field are mutually perpendicular, this Ising model has a quantum character and is often described as the simplest quantum mechanical model. The case of general a, b and c in (1) is usually called the Baxter XYZ model after BAXTER [19] who pioneered the analytic attack. These various solutions illustrate the special character of 1-D vs 3-D systems. Major features are the presence of characteristic rounded maxima in the specific heat and the perpendicular or antiferromagnetic parallel susceptibility. Such effects are attributed to short-range order since these systems show critical singularities only at $T = 0$. It should be noted, however, that if the interaction range is sufficiently increased, even 1-D model systems have critical points such that $T_c > 0$ [20].

Let us now review the analytic status of the general, spin-1/2 Ising-Heisenberg-XY linear chain with symmetry ($b = c$, say), often called the XXZ model. The mathematical analysis required for this general model is more complicated than that required to solve the 2-D Ising model (ONSAGER [21]). Since the 2-D Ising model solution has been so fruitful in the development of the modern theory of critical phenomena, it would seem profitable to pursue the 1-D quantum chain solution in equivalent detail. A breakthrough by YANG and YANG about 1966 [22] resulted in a detailed solution as a function of anisotropy and magnetic field for $T = 0$. However, this was sufficient to determine the character of the interesting critical singularities. The finite temperature properties presented a greater problem. Progress has been made by JOHNSON and McCOY [23] and JOHNSON [24], and independently by TAKAHASHI [25], on the basis of a formulation due to GAUDIN [26]. Nevertheless, information is still lacking, most notably for the Heisenberg ferro- and antiferromagnetic limits, and the correlation functions in general.

A parameter range of the XXZ model which has just yielded to analytic attack is the Ising-Heisenberg ferromagnet in zero and very small magnetic ffield. This corresponds to $a > b = c$ and $J > 0$ ln (1). For analytlc work, (1) is more conveniently written in the form

$$\mathcal{H} = -\sum_{i=1}^{N} \left\{ s_i^x s_{i+1}^x + s_i^y s_{i+1}^y + \Delta\left(s_i^z s_{i+1}^z - 1/4\right) \right\} - H \sum_{i=1}^{N} s_i^z. \tag{3}$$

Interesting and complex results have been obtained for the elementary excitations and low-temperature thermodynamics [27]. These results are based on the Bethe Ansatz (Gaudin formalism), and reveal complex cross-over behavior (a) as a function of spin anisotropy Δ and (b) as a function of magnetic field H. Fig. 1 shows the $H = 0$ excitations as a function of the anisotropy γ (the inverse of Δ). Near the Ising limit the thermal properties, e.g. specific heat, are dominated by the bound state excitation curve given by $E_B = \frac{1}{2}(\Delta^2 - 1)^{1/2}$ [i.e. $E_B/J = (1 - \gamma^2)^{1/2}$]. As the Heisenberg limit is approached, a cross-over occurs at $\gamma = 0.6$ ($\Delta = 5/3$) and thereafter the specific heat is dominated by a different class of excitations, unbound or spin wave in type, given by $E_{SW} = (\Delta - 1)$ [i.e. $E_{SW}/J = 2(1 - \gamma)$]. Interestingly, in the case of the magnetic excitations, i.e. susceptibility, domination by the bound states occurs over the whole anisotropy range from Ising to Heisenberg limits.

The situation is even more complicated when a field is applied. For sufficiently large fields, both χ and C_H are spin-wave dominated. For smaller fields (χ), and smaller fields with $\Delta > 5/3$ (C_H), there are two bound state dominated regions, between which cross-over occurs. These results are potentially interesting in connection with the quantum soliton problem, and to field theorists. Unfortunately, the important Heisenberg limit seems a more formidable problem, not tractable by

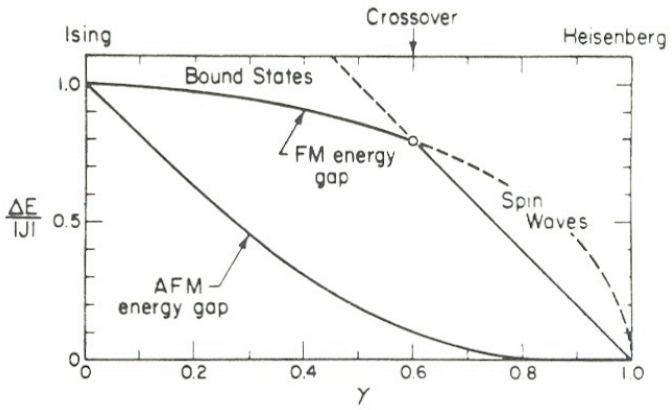

Figure 1. Cross-over behavior in the thermal excitations of the Ising-Heisenberg ferromagnet.

this method. Pioneering work is underway on two very different approaches which may be powerful enough to treat the Heisenberg limit (and find correlation functions). They are (a) the quantum inverse scattering method [28] and (b) a new and very abstruse approach pioneered by the Japanese [29].

Finally, mention should be made of a new approach which may be regarded either as an approximate treatment of a spin-1/2 1-D lattice or an exact treatment of a spin-1/2 1-D continuum model [30]. It is based on techniques for solving the field theoretic Tomonaga-Luttinger models [31]. The approach is now termed 'bosonization', and though quantitative accuracy is hard to assess, the general validity of the method has been established [32].

Bethe Ansatz Models and Mappings

The Bethe Ansatz was formulated in 1931 by BETHE [33] as a basic ingredient of the eigenfunctions of the Heisenberg spin 1/2 linear chain. The analytic results above for the general anisotropic and XYZ chains are all based on the Bethe Ansatz approach. Rather recently it was realized that the (generalized) Ansatz was the key to the analytic solution of a wider class of models than the quantum spin chain. Exact solutions came thick and fast for systems such as Fermi and Bose gas delta function models [34], the linear Hubbard model [35], 1-D plasma which crystallizes as a Wigner solid [36], and the Lai-Sutherland model [37] which includes the Hubbard model and a dilute magnetic model as special cases. Very recent work has mapped the Kondo problem into a 1-D Bethe Ansatz model whose solution is closely related to the problem of the Heisenberg spin chain [38].

A striking feature of current research is the large number of mappings or mathematical isomorphisms which have been discovered between the spin-1/2 quantum chain, including its various limiting cases, and a wide assortment of 1-D and higher-D models. Specifically, the mapping between 1-D quantum and 2-D classical models proceeds via the fact that the Hamiltonian matrix of the one class commutes with the transfer matrix of the other class (see XYZ proof by SUTHERLAND [38]). The various mappings have already been systematically reviewed in the context of soliton theory [40] and will simply be listed here. The general magnetic model of Hamiltonian (1) can be mapped into the following 2-D classical models: classes of ferro- and antiferroelectric models; classical Coulomb gas; 2-D Ising model; surface roughening model; the dimer problem [41]; lattice theories of polymer melting [41]; the percolation problem [42]; the coloring problem [42]; and the Potts model [43], under suitable special parameter choices and relevant parameter ranges. Hamiltonian (1) may also be mapped into the following 1-D models: the 1-D spinless fermion gas

with or without interactions; the 1-D quantum many-fermion Luttinger and Tomonaga models; generalised Hubbard-type models for organic conductors with hopping and on-site repulsive or attractive terms [44] [45], including the Hubbard dimer gas [46]. Note the Kondo problem solution represents essentially the first 1-D to 3-D mapping.

Finally we note that the mapping between 2-D classical vertex models and 1-D quantum models which can take place at zero or non-zero [47,48] temperature offers a radically new approach to the quantum chain problem. Unlike quantum systems, classical systems can be directly simulated on a computer and then the results can be transcribed to the quantum equivalents [49].

Quantum Spin Chains: Numerical Studies

The Bethe Ansatz approach to uniform spin chain problems applies only to quantum models with completely integrable Hamiltonians. This includes the spin-1/2 Heisenberg and XY models. It does not appear to be applicable to models with $S > 1/2$. Even for spin 1/2, the Bethe Ansatz approach cannot be applied to the Heisenberg alternating chain, a nearest-neighbor exchange model where there are two unequal exchange constants which alternate along the chain. Since the *alternating* chain is important to the theory of spin-Peierls transitions in quasi-1-D organics, and there is experimental interest in effective spin-1 systems (containing the Ni^{2+} ion), spin-3/2 systems (Cr^{3+} ion) and spin-5/2 systems (Mn^{2+} ion), reliable theoretical calculations are needed. Since an analytic approach is not feasible at this time, we must have recourse to a numerical BONNER-FISHER approach [50]. This involves calculating the properties exactly of a sequence of small finite spin chains, with both periodic and free-end boundary conditions, and steadily increasing system size N. Extrapolations are then made to the thermodynamic limit. The largest system in the sequence and hence number of systems available for extrapolation, is spin dependent, since the calculation involves symmetry reduction and subsequent diagonalization of Hamiltonian matrices of dimension $(2s+1)^N \times (2s+1)^N$. However, BLÖTE has been able to perform extrapolations for spin values $s = 1/2, 1, 3/2, 2$, up to 5/2, for ground state energies [51], specific heat [52], susceptibility, and $T = 0$ magnetization isotherms vs field [53]. The variation of specific heat (see [52]) and susceptibility (shown in Fig. 2) with spin is not very striking, except in one important respect. The $s = \infty$ curves all show non-physical features at low temperatures. For example, the classical Heisenberg specific heat [54] rises monotonically to a non-zero value as $T \to 0$, instead of vanishing in accordance with the third law of thermodynamics, as do the curves for $s < \infty$.

The accuracy of this extrapolation method, for the optimal case of spin 1/2, as estimated by comparison with subsequent analytically based calculations, is discussed in [1]. Ref. [1] also includes some detailed comparisons of the various quantum spin models.

Alternating Chains

Alternating spin chains are something of a novelty to physicists. Originally they were studied from a chemical viewpoint, to explain the properties of certain organic free radicals [55]. From such studies evolved spin-exciton theory [56]. Some recent applications have been to copper nitrate [57,58] and copper bromide imidazole [59]. Perhaps the most exciting application has been to members of a family of organometallic complexes, insulating relatives of the organic conductor TTF-TCNQ. These are the TTF bisdithiolenes, denoted TTF.BDT(M), where M = Cu or Au, the first experimental systems to display a spin-Peierls transition [60]. This is a magnetoelastic rather than purely magnetic phase transition. In zero field an assembly of Heisenberg, spin-1/2, uniform antiferromagnetic chains undergoes a transition as the temperature is lowered, as a result of lattice distortion. Below the transition the system is described as an assembly of alternating chains, where the degree of alternation is a function of temperature. The Hamiltonian for an

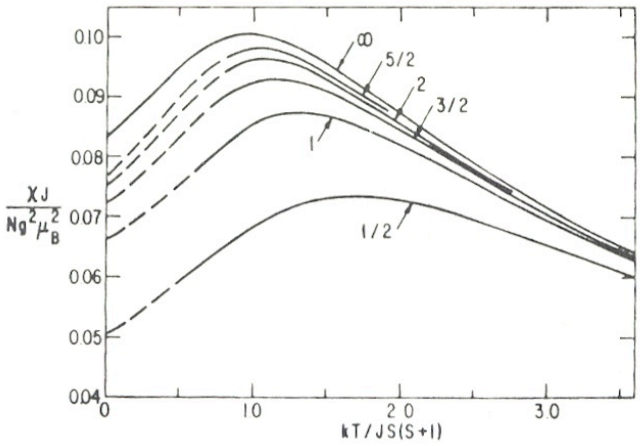

Figure 2. Extrapolated finite chain susceptibilities for Heisenberg antiferromagnets showing dependence on spin.

alternating Heisenberg chain may be written:

$$\mathcal{H} = -2J \sum_{i=1}^{N} \left\{ \vec{S}_{2i-1} \cdot \vec{S}_{2i} + \alpha \vec{S}_{2i} \cdot \vec{S}_{2i+1} \right\}, \tag{4}$$

where α is a convenient alternation parameter, i.e. the ratio of interaction strengths of the two exchange constants. When $\alpha = 0$, the alternating chain reduces to a non-interacting assembly of spin-pairs or dimers (dimer limit). When $\alpha = 1$, we recover the familiar uniform Heisenberg chain of (2).

In the absence of some generalized Ansatz serving as a basis for analytical attack, this model has been treated theoretically by a variety of approximate techniques. Two of the more successful methods are the BULAEVSKII Hartree-Fock approach [61] subsequently incorporated into spin-Peierls theory by PYTTE [62] and BRAY ET AL. [63]; and an alternating variant of the LUTHER-PESCHEL-LUTTINGER continuum model [30], employed in the spin-Peierls work of CROSS and FISHER [64]. There are differences between them, and the Luttinger approach, which is not a mean-field approach, is claimed to have greater accuracy. However, there is at present no available experimental means of distinguishing between the two models. Hence an extensive numerical finite chain study was undertaken on periodic alternating chains of up to 12 spins [65] in an attempt to extend earlier studies by DUFFY and BARR [55]. Attention was paid both to spectral excitations and thermodynamic properties. A comparative study of extrapolated susceptibilities over the entire a range vs calculations based on the Bulaevskii paper [66] has already appeared. The behavior of the $T = 0$ magnetization isotherms as a function of a is shown in Fig. 3. In general, we remark that in comparison with the more exact calculations the mean-field Bulaevskii theory is surprisingly successful. No spurious $T > 0$ phase transition appears for antiferromagnetic systems. Thermodynamic predictions are qualitatively correct but quantitatively in error by roughly 15% over the whole alternation range. No similar direct comparisons can be made with the CROSS-FISHER theory [64], since at present a Luttinger-type approach cannot predict amplitudes, which are cut-off dependent and therefore arbitrary.

The numerical calculations strongly suggest that the presence of alternation results in the appearance of an energy gap between the non-degenerate singlet ground state and the lowest excited states (triplet excitons), i.e. the gap vanishes only in the uniform limit, $\alpha = 1$. Fig. 4 shows finite N curves for alternating chains of 2 through 12 spins, together with the extrapolated result,

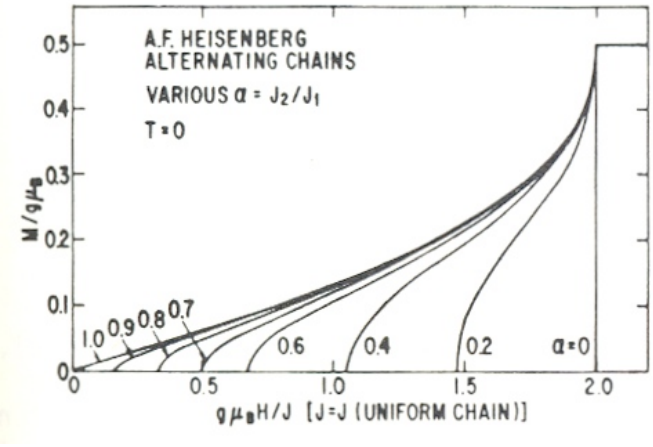

Figure 3. Zero-temperature magnetization isotherms for alternating Heisenberg linear antiferromagnet.

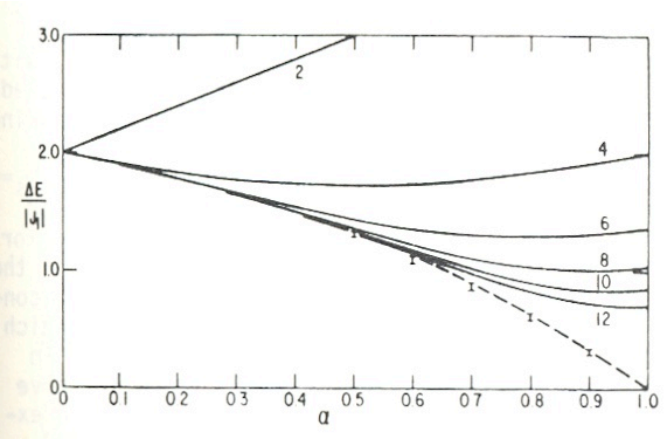

Figure 4. Finite chain extrapolation for energy gap of alternating linear Heisenberg anti ferromagnet.

and results of BULAEVSKII [61] for comparison. The existence of such a gap is crucial to spin-Peierls theory and also spin exciton theory in physical chemistry. However, since the alternating linear chain still possesses full isotropic spin symmetry, doubts have been raised on the basis of intuition derived essentially from classical (spin-∞) 1-D systems, about the existence of such a gap [67]. It is interesting that the XY alternating chain, which can be solved exactly for both $s = 1/2$ and $s = \infty$, shows a gap in the quantum case and no gap in the classical case, for all non-zero alternation. Numerical evidence is very strong that the same situation occurs for the Heisenberg antiferromagnetic alternating chain.

Quantum Renormalization Group Method

The real space renormalization group (RG) method pioneered by NIEMEIJER and VAN LEEUWEN [68] has been very successfully applied to 1-D [69] and 2-D [70] Ising models. However, a successful real space RG method for quantum systems has been slow in coming, essentially because of the familiar problem of non-commuting operators. A new method devised recently by field theorists [71] and shortly thereafter applied to a type of Kondo problem [72], offers hope. The class

of quantum spin models provides obvious test cases for the new method, which will be reviewed in this light. We note again that the lack of exact solutions for uniform chains with $1/2 < s < \infty$ and alternating chains with $s < \infty$ makes reliable approximate methods valuable.

The spirit of the method is as follows. The lattice is sub-divided into blocks of N_s sites such that the eigenvalues and eigenvectors of each block may be calculated exactly. The basis of each block ($2^N s$ levels, $s = 1/2$) is truncated to some number N_L of levels, and the coupling between the blocks is written within the truncated basis. If the temperature region of interest is $T = 0$, where the critical singularities are located for 1-D, short-range, quantum models, then the truncated basis need only contain the ground state and dominant set of first excited states. If, therefore, both N_s and N_L are small, analytic RG recursion relations can be formulated and solved. In general, however, use of a computer is required. This is true if information at higher temperatures is needed. High temperature calculations may use directly all the block levels instead of just the lowest [73], or may use an approximate technique which preserves the important information contained in the higher levels at each recursion step [74].

The new method has been exhaustively tested on the simplest quantum model the transverse Ising model, with encouraging results [71,75]. A more stringent test is posed by the more complex quantum models like the 1-D alternating Heisenberg anti ferromagnet and the 1-D Ising-Heisenberg spin-anisotropic antiferromagnet (Eq.(1) with $a > b = c$ and $J < 0$). Comparison can be made with finite chain calculations and, in the case of the Ising-Heisenberg chain, with exact analytic results [77,76,23]. In Fig. 5a, we see again the extrapolated finite chain energy gap ΔE for Heisenberg antiferromagnetic alternating chains together with the exact result for $N = 12$. In comparison we see the energy gap predictions for two types of RG calculation. One curve corresponds to N (odd) with $N_L = 2$, giving an unstable fixed point at $\alpha^* = 1$ (uniform limit) and a stable fixed point at $\alpha^* = 0$ (dimer limit), consistent with an energy gap for all $\alpha < 1$, in agreement with numerical predictions. However, the value of gap is quantitatively unreliable near the dimer limit (where finite chain convergence is excellent). This is attributable to the 2-level truncation which does not utilize the singlet-triplet character of the low-lying levels. In comparison we show an $N_s = 4$ (even), 4-level truncation RG which does preserve the singlet-triplet symmetry. This RG is in very good agreement with the extrapolated curve out to $\alpha \simeq 0.6$, but predicts a gap vanishing at $\alpha = 0.962$ rather than unity. This must be interpreted as resulting from automatic failure of an important symmetry ($\alpha \leftrightarrow \alpha^{-1}$) whenever N_s is even. In Fig. 5b, c comparable results for the Ising-Heisenberg antiferromagnet with spin anisotropy parameter $\gamma = b/a$ are shown. Crosses show the energy gap obtained by extrapolation of the finite chain sequence $N = 4, 6, 8, 10, 12$. The extrapolations predicted that the gap vanished only at $\gamma = 1$ [50], a prediction confirmed by subsequent analytic calculations [76,23] which gave a gap (solid curve) vanishing exponentially as $\gamma \to 0$. An $N_s = 3$, $N_L = 2$ RG result (dashed) is characterized by fixed points $\gamma^* = 1$ (unstable) and $\gamma^* = 0$ (stable), and hence vanishes at $\gamma = 1$. However the curve is clearly in poor agreement with the exact result. Finite temperature properties using this method have been obtained by JOSÉ and HIRSCH [74] in the context of a study of random anisotropic anti ferromagnet chains. The accuracy of the method was tested for the limiting case of the uniform Heisenberg chain by comparison with numerical extrapolations [50]. For both specific heat and susceptibility, agreement was fair over most of the temperature range (i .e. to within 15-20%). There is a more serious problem at very low temperatures. It appears that the fundamental structure of these RG's may lead to non-physical behavior. Specifically, the susceptibility vanishes instead of going to a finite limiting value known exactly [78] and the specific heat vanishes with zero slope instead of linearly [23,50].

Quantities which can be regarded as critical singularities for the spin-Peierls problem are (a) the value of deviation of the ground state energy per spin from its exactly known [79] uniform value with the onset of dimerization (call this ξ_0) and (b) quantitatively how the energy gap between ground and first excited states (ΔE) behaves near the uniform limit as a function of alternation. Predictions of the various approximate methods are collected in Table 1. In order to obtain analytic results, the finite chain extrapolations have been augmented by RG based finite

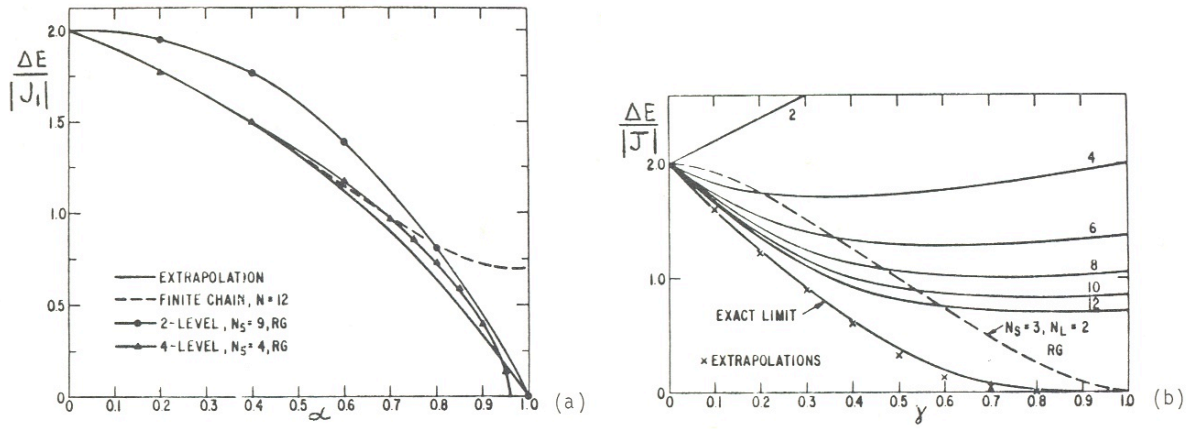

Figure 5. (a) N_s odd and even RG calculations in comparison with extrapolated result for alternation energy gap. (b) Finite chain extrapolations and RG calculation for Ising-Heisenberg anisotropy energy gap compared with exact result.

size scaling techniques [80]. A point of interest is the difference between the analytic finite chain exponents and the analytic Cross-Fisher exponents which are claimed to be exact [64].

Table 1. Comparison of spin-Peierls exponents.

Method	Ground State Energy	Energy Gap
Hartree-Fock [69]	$\xi_0 \sim \delta^2(\ln\delta)^2$	$\Delta E \sim \delta \ln\delta$
Cross-Fisher [72]	$\xi_0 \sim \delta^{4/3}$	$\Delta E \sim \delta^{2/3}$
N_{odd} RG [77]	$\xi_0 \sim \delta^{1.5}$	$\Delta E \sim \delta^{0.76}$
N_{even} RG [77]	$\xi_0 \sim \delta^{1.6}$	$\Delta E \sim \delta^{0.64}$
Finite Chains [80]	$\xi_0 \sim \delta^{3/2}$	$\Delta E \sim \delta^{3/4}$

Quantum Spin Dynamics

Spin dynamical calculations on 1-D systems have relied heavily on classical ($S = \infty$) theory [9,10,11] despite abundant evidence that quantum effects can be extremely important at low temperatures. A new approach to the spin dynamics of the 1-D isotropic $S = 1/2$ Heisenberg anti ferromagnet [81-83] does not involve the many-body techniques usually employed, but instead is based on analytic calculations of excitation energies and densities of states combined with finite chain calculations of matrix elements. Specifically the results are obtained on the basis of four main techniques: (1) analytic calculations of a special class of Bethe-Ansatz states; (2) exact finite chain calculations for chains of 4 through 10 spins; (3) derivation and application of two different kinds of selection rules; and (4) the use of various kinds of sum rules. Major emphasis has been put on zero-temperature studies in zero and non-zero field. Finite chain calculations have been used to extend the dynamical study to finite temperatures.

In zero field an approximate analytic expression is available for the dynamical correlation function which fits excellently into the fragmentary picture of the few available exact results. This expression has then been exploited to yield a variety of further results of theoretical and experimental interest. The $T = 0$ expression is governed by a two-parameter continuum of spin-wave-type

triplet ($s = l$) excitations. Explicitly,

$$S_{\mu\mu}(q,\omega) = \frac{A}{\left[\omega^2 - (\pi J/2)^2 \sin^2 q\right]} \Theta\left(\omega - \frac{1}{2}\pi J|\sin q|\right) \Theta\left(\pi J \left|\sin\frac{q}{2}\right| - \omega\right). \tag{5}$$

This expression 'switches on' at the lower continuum boundary given by the formula $E_1(q) = (\pi J/2)|\sin q|$ (first derived by DES CLOIZEAUX and PEARSON [84]), where there is a divergence. A tail of decreasing spectral weight extends to the upper continuum boundary, $E_2(q) = \pi J|\sin(q/2)|$, where there is a cut-off, dependent on the value of the constant A. This expression is not rigorous, but exact sum rules are violated by only a small amount. Expression (5) predicts increasing asymmetry in the spectral weight distribution as $q \to \pi$, a purely quantum effect, which has recently been verified by neutron scattering data [85]. The result for the integrated intensity derived from (5) is in much better agreement with neutron scattering data on the linear chain antiferromagnet cobalt chloride dipyridine (CPC) [86] than the corresponding semi-classical result.

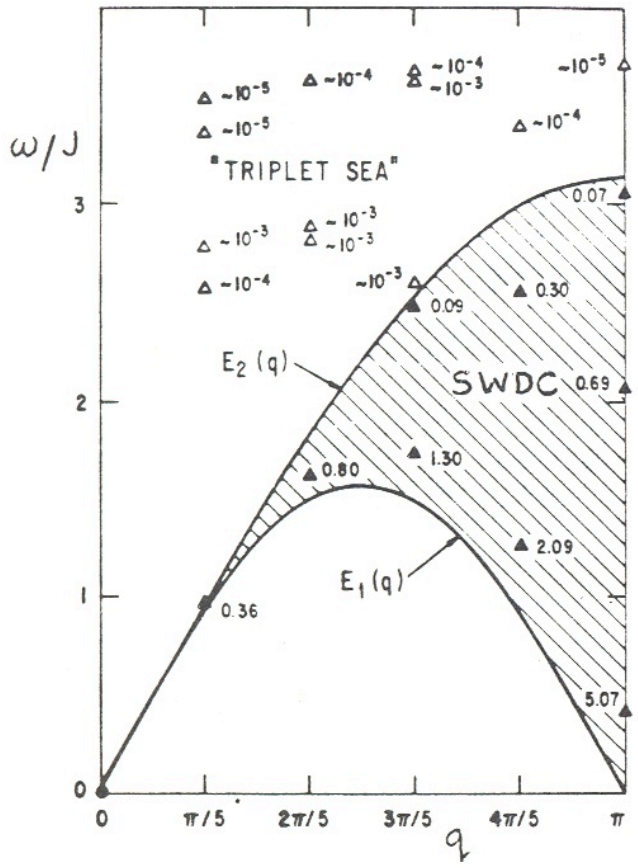

Figure 6. Exact calculation. of $S_{zz}(q,\omega)$ for a chain of $N = 10$ spins in zero field.

In Fig. 6 we show an exact calculation of $S_{zz}(q,\omega)$ for a cyclic chain of $N = 10$ spins. For each q, $S_{zz}(q,\omega)$ is a collectlon of δ functions. The triangles denote energy and wave number of the triplet excitations, and the numbers represent the corresponding spectral weight. No type of excitation other than triplet carries any spectral weight. We may note the following: (a) almost all the spectral weight is concentrated within the boundaries of the spin-wave double continuum (SWDC); (b) the matrix elements increase in magnitude as the energy decreases to the lower boundary $E_1(q)$ (and also increase in magnitude as $q \to \pi$); and (c) there is some very small but finite weight above $E_2(q)$. Exact sum rule arguments of HOHENBERG and BRINKMAN [87]

and finite chain calculations [88] indicate that this weight should persist in the thermodynamic limit. Some interesting information is available on states of this type near the critical field, which calls for further investigation of their nature for all fields. The value of the constant A may be approximately determined from sum rules. Three simple sum rules link $S_{zz}(q,\omega)$ to the static susceptibility, the ground state energy, and the integrated intensity. The resulting values for A differ among themselves by about 20% with a mean of $A \simeq 1.18$, reflecting failure to take account of states of the 'triplet sea'.

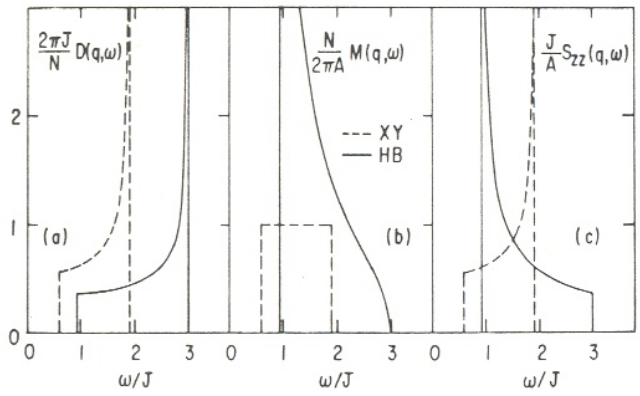

Figure 7. Comparison of $T = 0$ density of state functions, matrix element functions, and dynamical correlation functions for Heisenberg vs XY models.

Fig. 7 shows an interesting comparison between Heisenberg and XY models at $T = 0$ for density of states $D(q,\omega)$; matrix element function $M(q,\omega)$; and dynamical correlation function $S_{zz}(q,\omega)$. For both models $D(q,\omega)$ diverges at the upper SWDC boundary. The XY matrix elements are constant over the SWDC, but diverge strongly at the lower boundary for the Heisenberg model. Hence we have the interesting difference between the models that $S_{zz}(q,\omega)$ diverges at the *lower* boundary for the Heisenberg model but at the *upper* boundary for the XY model.

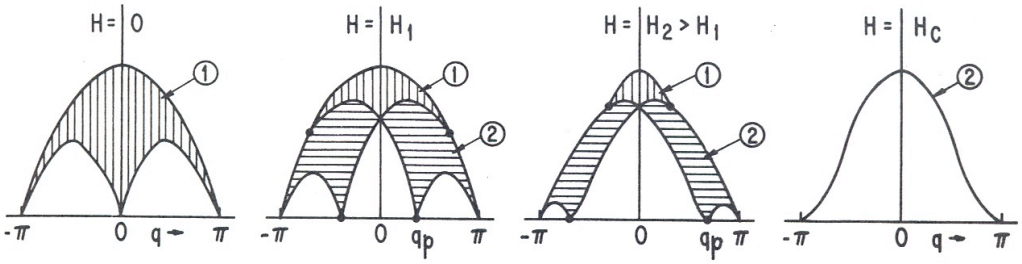

Figure 8. Behavior of the two continua dominating $S_{zz}(q,\omega)$ as a function of magnetic field.

For non-zero field there are striking differences between the longitudinal and the transverse correlations, both involving different continua of excitations. With increasing field, the longitudinal fluctuations are more and more suppressed, whereas the transverse fluctuations become more important. Exact selection rules show that for $H = 0$ and finite N, six different SWDC contribute to the dynamics, two for the longitudinal and four for the transverse correlations, giving rise to considerable complexity. In Fig. 8 the behavior of the two continua for $S_{zz}(q,\omega)$ is shown as a function of H. As H increases, the importance of contlnuum 1 decreases. It is most interesting that in the thermodynamic limit it may be proved that additional selection rules come into play, reducing the number of contributing continua from 6 to 3. In Fig. 8, continuum 1 loses all weight

for $H > 0$ in the limit leaving only continuum 2. In zero field, however, continuum 1 continues to dominate exclusively!

The theory for $H > 0$ predicts multiple structures in the scattering intensity, various features of $S_{zz}(q,\omega)$ and $S_{xx}(q,\omega)$ which are simply related to the magnetic field, e.g. soft mode locations and energy relations between scattering peaks, and quite different behavior for the corresponding integrated intensities, $I_{zz}(q)$ and $I_{xx}(q)$. All these features are susceptible to future experimental observation.

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