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Density matrix renormalization group study of the correlation function of the bilinear–biquadratic spin-1 chain

R J Bursill†§, T Xiang‡ and G A Gehring†

† Department of Physics, The University of Sheffield, Sheffield S3 7RH, UK

‡ Interdisciplinary Research Centre in Supeconductivity, The University of Cambridge, Cambridge CB3 0HE, UK

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Abstract. Using the recently developed density matrix renormalization group approach, we study the correlation function of the spin-1 chain with quadratic and biquadratic interactions. This allows us to define and calculate the periodicity of the ground state which differs markedly from that in the classical analogue. Combining our results with other studies, we predict three phases in the region where the quadratic and biquadratic terms are both positive.

1. Introduction

The application of the real space renormalization group (RSRG) to quantum lattice models [1] has received renewed interest in recent times due to the development of the density matrix renormalization group (DMRG) by White and co-workers [2]. DMRG studies of the spin-1 chain with pure antiferromagnetic exchange [3, 4] yielded ground-state properties with unprecedented reliability and accuracy. Applications to coupled spin [5] and Hubbard [6] chains have followed and applications to fermion systems in two dimensions are being pursued [7].

The spin-1 chain has been the subject of much recent interest because of theoretical predictions [8] and experimental observations [9] of a gap in the excitation spectrum of integer spin Heisenberg models, verified beyond doubt in the spin-1 case in [3].

In this paper we present results from the application of the DMRG to a generalization of the standard spin-1 chain where a biquadratic interaction is added to the usual Heisenberg exchange, i.e.

$$\mathcal{H} = \sum_i \left[\cos\gamma\, S_i \cdot S_{i+1} + \sin\gamma (S_i \cdot S_{i+1})^2\right] \tag{1.1}$$

where S_i is the spin-1 operator for site i and γ is a parameter determining the relative strength of the bilinear and biquadratic interactions. We concentrate on the regime $0 \leqslant \gamma \leqslant \pi/2$ where the quadratic term is antiferromagnetic and the biquadratic term opposes any kind of order between neighbours.

As mentioned, in the $\gamma = 0$ case the existence of a gap Δ (between the spin-0 ground state and the spin-1 first excited state) has been well established. Also calculated in [3] is the spin–spin correlation function

$$C(i-j) = \langle S_i^z S_j^z \rangle \tag{1.2}$$

§ E-mail: r.bursill@sheffield.ac.uk

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which is found to decay exponentialy with alternating sign, being well fitted by

$$C(r) \sim A\frac{(-1)^r e^{-r/\xi}}{r^{1/2}} \tag{1.3}$$

with correlation length $\xi \approx 6.03$. The ground state is disordered in the conventional sense although an interesting type of topological long-range order, characterized by a *string order parameter*

$$g(l) \equiv \left\langle S_0^z \left(\prod_{j=1}^{l-1} e^{i\pi S_j^z} \right) S_l^z \right\rangle \tag{1.4}$$

exists and has been calculated [3].

For $\gamma = \arctan\frac{1}{3}$ the ground-state wavefunction can be written down [10], having a simple valence-bond solid structure. The ground-state energy is known exactly and a gap to the first excited ($S = 1$) state can be shown to exist. The correlation function is given by

$$C(r) = \tfrac{4}{3}(-1)^r 3^{-r} \qquad \text{for } r > 0 \tag{1.5}$$

so that $C(r)$ again decays exponentially with alternating sign and has correlation length

$$\xi = 1/\log 3 = 0.9102\ldots. \tag{1.6}$$

At $\gamma = \pi/4$ the model is exactly solvable by the Bethe ansatz [11], the excitation spectrum being gapless and having soft modes at 0 and $\pm 2\pi/3$. In this case standard field theory predicts that $C(r)$ should decay algebraically. This suggests that a phase transition occurs at $\gamma = \gamma_c \in (\arctan\frac{1}{3}, \pi/4]$ where the correlation length diverges.

Two of us (TX and GAG) have studied the ground-state energy density ϵ_G of (1.1) using a variant of the RSRG [12]. It was noticed qualitatively that there was a crossover from conventional antiferromagnetic period-2 behaviour to period-3 behaviour in the (weak) chain length dependence of ϵ_G as γ was varied between 0 (the Heisenberg point) and $\pi/4$ (where, as a result of the soft mode at $2\pi/3$, a triply periodic ground state in expected). It was found that the crossover occurred near $\gamma = 0.15\pi$ though we emphasize that this observation was only qualitative.

The following questions thus arise naturally:

(i) Is $\gamma_c = \pi/4$?

(ii) What are the exponents which characterize the divergence of the correlation length and the subsequent algebraic decay of $C(r)$?

(iii) Does Δ vanish for $\gamma \geqslant \gamma_c$?

(iv) What is a good definition of the *periodicity* of the ground state?

(v) How does the periodicity vary with γ?

(vi) Is there a relationship between the periodicity and the classical pitch angle θ^* (the angle between sucessive spins in the ground state of the classical ($S = \infty$) analogue)?

(vii) How should the string order parameter be defined (for general γ) and what is its value?

The above questions have been the subject of both analytical [13–15] and numerical [16–20] studies, often with conflicting results.

Though there are no completely firm answers to any of the above questions, the most definitive study of (1.1) is the most recent study by Fáth and Sólyom [17] where finite-size scaling and twisted boundary condition techniques are applied in analysing exact results from small chains. The answer to question (i) is found to be in the affirmative, there being a transition of the Kosterlitz–Thouless type at $\gamma = \gamma_c = \pi/4$. It is also found, in answer to

question (iii), that Δ does indeed vanish for $\gamma_c \leqslant \gamma \leqslant \pi/2$. The exponent σ, characterizing the opening of the gap, is also estimated.

As mentioned, the questions concerning the periodicity of the ground state were qualitatively addressed in [12]. They were also studied qualitatively in [16] where again evidence of a triply periodic ground state was found for $\pi/4 \leqslant \gamma \leqslant \pi/2$ and also in a region below $\pi/4$. This agrees qualitatively with analyical predictions from spin wave [14] and variational [15] theories.

In this paper we attempt to answer (iv)–(vi) quantitatively by calculating (1.2) using the DMRG. The DMRG allows us to study much longer chains than those studied in [16, 17]. This facilitates the accurate calculation of $C(r)$ for r up to around 50 and hence its Fourier transform

$$\tilde{C}(q) \equiv \sum_r C(r)e^{iqr}. \tag{1.7}$$

We are then able to define and calculate the periodicity of the ground state in terms of the position where $\tilde{C}(q)$ has its peak.

In the next section we describe our implementation of the DMRG for (1.1) and our results for $C(r)$ and the periodicity of the ground state.

2. DMRG results for the spin–spin correlation function

2.1. The DMRG method for spin chains

As mentioned, the DMRG was introduced in a series of papers [2] where efficient algorithms for calculating low-lying energies and correlation functions of spin chains are described in great detail. We will therefore be very brief in our description of the method. We restrict our discussion to the infinite lattice algorithm [2] which we used for our calculations.

The DMRG is an iterative, truncated basis procedure whereby a large chain (or superblock) is built up from a single site by adding a small number of sites at a time. At each stage the superblock consists of system and enviroment blocks (determined from previous iterations) in addition to a small number of extra sites. Also determined from previous iterations are the matrix elements of various operators such as the block Hamiltonians and the spin operators for the sites at the end(s) of the blocks) with respect to a truncated basis. Tensor products of the states of the system block, the enviroment block and the extra sites are then formed to provide a truncated basis for the superblock. The ground state $|\psi\rangle$ (or other targeted state) of the superblock is determined by a sparse matrix diagonalization algorithm.

At this point, correlation functions, local energies and other expectation values are calculated with respect to $|\psi\rangle$. Next, a basis for an augmented block, consisting of the system block and a specified choice of the extra sites, is formed from tensor products of system block and site states. The augmented block becomes the system block in the next iteration. However, in order to keep the size of the superblock basis from growing, the basis for the augmented block is truncated. We form a density matrix by projecting $|\psi\rangle\langle\psi|$ onto the augmented block which we diagonalize with a dense matrix routine. We retain the *most probable* eigenstates (those with the largest eigenvalues) of the density matrix in order to form a truncated basis for the augmented block that is around the same size as the system block basis. Matrix elements for the Hamiltonian and active site operators, together with any other operators that are required for say, correlation functions are then updated.

The environment block used for the next iteration is usually chosen to be a reflected version of the augmented block. The initial system and environment blocks are chosen to

be single sites.

We note that the key parameter determining the accuracy and, correspondingly, the computer requirements (both CPU time and memory) is n_s, the number of states retained per block (of good quantum numbers) at each iteration. n_s therefore determines the truncation error, which is the sum of the eigenvalues of the density matrix corresponding to states which are shed in the truncation process. A large truncation error indicates that too many important states are being shed and that n_s is too small. The error in quantities such as the ground-state energy scale linearly with the truncation error [3].

The application of the DMRG to the spin-1 chain with pure antiferromagnetic nearest-neighbour exchange ($\gamma = 0$) is described in detail in [3]. We will not repeat this description here, rather we describe the results of our extension of the method to $\gamma \neq 0$, paying attention to particular difficulties that arise in this case.

2.2. *Application of the* DMRG *to the bilinear–biquadratic chain*

We have applied the infinite-lattice DMRG algorithm to the calculation of $C(r)$ for (1.1) using a number of superblock configurations and boundary conditions. All the interactions (intrablock, interblock and superblock Hamiltonians) commute with the total z spin $S_T^z \equiv \sum_i S_i^z$, so S_T^z is a good quantum number which can be used to block diagonalize the system, environment and super blocks. The ground state of the superblock $|\psi\rangle$ is a singlet with zero total spin so we only need to consider superblock states with $S_T^z = 0$.

With the computing power available to us (14 megaflop Silicon Graphics Indigo II workstation with 80 Mbyte of free memory) we found that the most CPU efficient configuration was an open ended superblock of the form system–site–enviroment. We gauged the efficiency of a given configuration by assessing how rapidly the ground-state energy density, a by-product of the calculation, converged to its known value in cases where exact values or high-precision numerical results are available.

With $n_s = 40$, a calculation for the $\gamma = 0$ case involving 49 iterations (99-site superblock) takes around 14 hr of CPU time and requires around 5 Mbyte of memory. With $n_s = 50$ for $\gamma = \pi/4$, 250 iterations took up 10 days of CPU time. In general the resource requirements increase as the square of n_s. We next describe the attainable accuracy which, as we shall see, depends strongly on γ through the excitation gap and rate of decay of the correlation functions.

2.3. *Testing of the method*

Ground-state energy density

We calculate ϵ_G by evaluating the local energy [3]:

$$\cos\gamma\, S_i \cdot S_{i+1} + \sin\gamma (S_i \cdot S_{i+1})^2 \tag{2.1}$$

where i is a site in the middle of the superblock (i.e. the end site of the system block). This reduces the end effects considerably. For a given choice of n_s the scheme is iterated until this quantity converges. The local energy is calculated for various values of n_s and the error is estimated using the proportionality of the error to the truncation error [3].

(i) Haldane point ($\gamma = 0$). In this case the ground-state energy density is known to high precision (at least seven significant figures) from the large-scale DMRG calculation using careful smoothing of the boundary conditions [3] which has been verified independently by a very large-scale exact diagonalization and finite-size scaling analysis [21]. In our

implementation, agreement to seven significant figures can be reached using $n_s = 40$ and around 50 iterations are required for the local energy to converge to this accuracy.

(ii) Affleck point $\tan\gamma = 1/3$. As mentioned, the ground-state wavefunction has a simple, known structure and the exact ground-state energy density is known. With $n_s = 40$ we recover the ground-state energy density to within round-off error after only a few iterations. This is due to the fact that the ground state can be built up exactly by retaining only a few states at each iteration.

(iii) Lai–Sutherland point $\gamma = \pi/4$. As mentioned, the energy spectrum in this case is gapless and the correlations are predicted to decay algebraically. These two conditions are very unfavourable for accurate DMRG calculations [2] (convergence is algebraic rather than exponential in n_s if the spectrum is gapless) and this is borne out in our implementation. That is, with $n_s = 50$ we achieve agreement with the exact ground-state energy density only to within one-tenth of 1%. The Lai–Sutherland point is critical so boundary effects are strong and around 250 iterations are required to achieve convergence of the local energy to four significant figures.

Table 1. Estimates of the ground-state energy density ϵ_G from the DMRG and exact or precise results.

$\tan\gamma$	DMRG	Exact
0	−1.401 484 5(38)	−1.401 484 03...
1/3	0.666 666 666 667(1)	2/3
1	0.2963(8)	0.296 78...

Table 1 shows the DMRG ground-state energy density together with the exact or precise result for the three cases mentioned above. In each instance the exact or precise result was recovered within the error bound calculated from the truncation error.

Finite chains

We also tested the algorithm for finite chains by calculating the exact ground-state energy and correlation functions for small chains (of up to 13 sites) by the Lanzcos method and ensuring that the DMRG recovered the exact result.

2.4. Results for the correlation function

To calculate the correlation functions we retain and update the matrix elements of the S_i^z for i near the active end of the blocks at each iteration. This is the part of the calculation that uses the bulk of the CPU and memory resources. We calculate $C(r)$ by evaluating $\langle\psi|S_i^z S_j^z|\psi\rangle$ for $j - i = r$, where i and j are sites equidistant from the centre of the superblock [3] (again to minimize end effects and optimize convergence).

There are two sources of error in calculating $\tilde{C}(q)$—truncation of the Hilbert space and truncation of the Fourier series. In forming the Fourier transform (1.7) we use the Fourier coefficients $C(r)$ which converge to at least two significant figures. The convergence rate of $C(r)$ with lattice size decreases with r because the number of truncations performed on the spin matrices used to form $C(r)$ increases linearly with r. The first few coefficients have a similar dependence on n_s (or the truncation error) to the ground-state energy density. For $r \gtrsim 10$ errors due to spin matrix truncation, rather than truncation of $|\psi\rangle$, begin to become dominant.

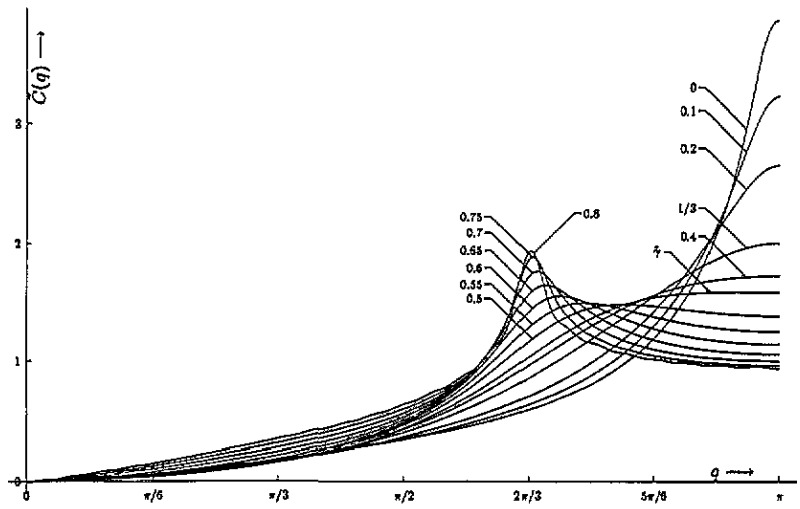

Figure 1. $\tilde{C}(q)$ against q for various values of γ.

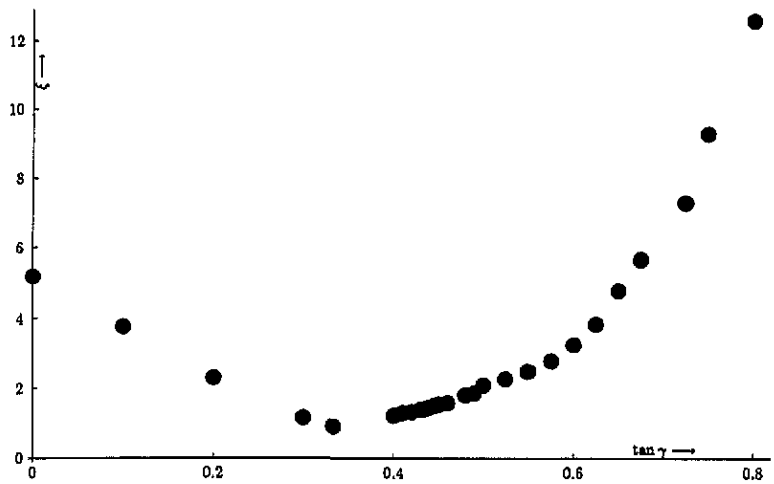

Figure 2. Estimate of the correlation length ξ for various values of γ.

Plots of $\tilde{C}(q)$ against q for various values of γ using $n_s = 40$ are given in figure 1. At the Haldane point $\tilde{C}(q)$ is peaked sharply around $q = \pi$ as is to be expected from strongly period-2 behaviour. As γ is increased, the width of the peak increases. At some point $\gamma = \tilde{\gamma}$ the peak begins to move away from π towards $2\pi/3$ as γ is increased towards $\pi/4$, the Lai–Sutherland point, where period-3 behaviour is expected. The peak sharpens as γ approaches $\pi/4$ consistent with the algebraic decay predicted in $C(r)$ at $\gamma = \pi/4$.

Estimates of the correlation length

In figure 2 we give a crude estimate of the correlation length ξ obtained simply by linearly

fitting $\log|C(r)|$ over around 20 sites. This procedure is meaningful if $\tilde{C}(q)$ has a strong peak at π. The procedure can also be made more explicit if $\tilde{C}(q)$ has a strong peak at or near $2\pi/3$. For example, for $\tan\gamma = 3/4$, $\tilde{C}(q)$ has a peak at $0.6718(4)\pi$. $C(r)$ is plotted as a function of r in figure 3 where we see strong triply periodic behaviour. Plots of $\log|C(3r)|$, $\log|C(3r+1)|$ and $\log|C(3r+2)|$ are given in figure 4. The slopes of the three curves are roughly equal and the fitting procedure yields the result of taking the average of these slopes.

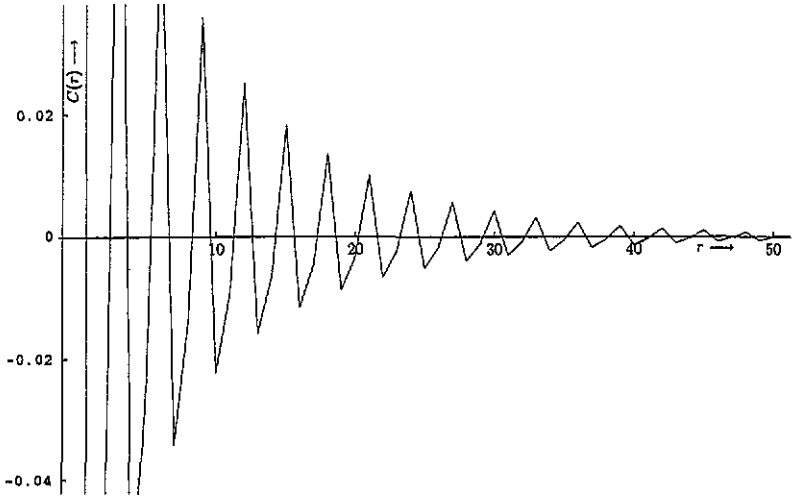

Figure 3. The correlation function $C(r)$ in the case where $\tan\gamma = 3/4$.

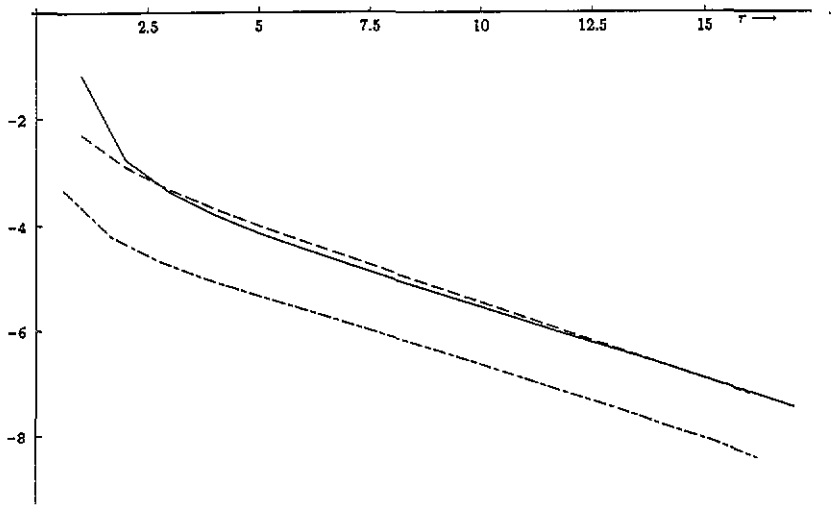

Figure 4. $\log|C(3r)|$ (full curve), $\log|C(3r+1)|$ (broken curve) and $\log|C(3r+2)|$ (chain curve) in the case where $\tan\gamma = 3/4$.

ξ estimated in this way depends weakly on range of sites over which the average is taken, though in general significant systematic error is expected due to Hilbert space truncation in addition to error in not taking into account the (generally unknown) correct

asymptotic form of $C(r)$. At the Haldane point (with $n_s = 40$) we get $\xi \approx 5.2$—only 87% of its precise value 6.0... [3] which was obtained from a very large-scale calculation, assuming and taking into account the extra algebraic factor in the asymptotic form (1.3). At the Affleck point we recover the exact correlation length to five significant figures though this is again due to the simplicity of the wavefunction.

For $0 \leqslant \tan\gamma \lesssim 3/4$, $C(r)$ decays exponentially and the error due to truncation of the Fourier series is negligible. For $3/4 \lesssim \tan\gamma \leqslant 1$ the correlation length is large and there is significant oscillation in $\tilde{C}(q)$ due to Fourier series truncation. This can be seen in figure 1 in the $\tan\gamma = 0.8$ case. For $\gamma \geqslant \pi/4$, $C(r)$ appears to decay algebraically and the peak appears to remain precisely at $2\pi/3$. This is consistent with previous numerical studies [16] where gapless excitations with soft modes at $\gamma = 0, \pm 2\pi/3$ are found and it is conjectured that the model is critical and triply periodic in the whole region. Our crude estimates of ξ in the region $0 \leqslant \tan\gamma \leqslant 0.8$ are consistent with the prediction of [17] that $\gamma_c = \pi/4$ and hence that ξ should diverge as $\gamma \to \pi/4^-$.

Peak position and periodicity of the ground state

From the above discussion we are led to the natural (working) definition of the ground-state periodicity, namely $2\pi/q^*$, where q^* denotes the position where $\tilde{C}(q)$ has its peak. The peak position converges quite rapidly with n_s and also with n_F, the number of converged Fourier coefficients retained, in cases where Fourier series truncation is not negligible. In table 2 we list q^* for various values of n_F and n_s for the case where $\tan\gamma = 3/4$.

Table 2. Convergence of the peak position q^* for the case where $\tan\gamma = 3/4$.

n_s	n_F	q^*
20	20	0.676 10
20	30	0.673 62
20	40	0.673 14
20	50	0.672 85
30	20	0.675 52
30	30	0.673 01
30	40	0.672 38
30	50	0.671 95
40	20	0.675 26
40	30	0.672 75
40	40	0.672 21
40	50	0.671 82

In figure 5 we plot q^* as a function of γ. As mentioned above, the ground state seems to be triply periodic in the whole region $\pi/4 \leqslant \gamma < \pi/2$. The fluctuations of q^* about $2\pi/3$ are around half of 1%, which is within the error that can be estimated from the rate of convergence. This is in agreement with predictions from spin wave [14] and variational [15] theories.

We see that the periodicity seems to be very close to 3 in the region $0.225\pi \lesssim \gamma \leqslant \pi/2$. It is not clear from our data whether q^* lies strictly above $2\pi/3$ in the whole open interval $0 < \gamma < \pi/4$ or not. Significantly higher precision in q^* would be required to decide this.

Next we consider the point $\gamma = \tilde{\gamma} \approx 0.13\pi$, beyond which the periodicity is greater than 2. In the vicinity of $\tilde{\gamma}$ the correlation length is very short and convergence of q^* with n_s is very rapid. The error (between our best result and results for smaller n_s) is roughly proportional to the truncation error. As with the ground-state energy density, we

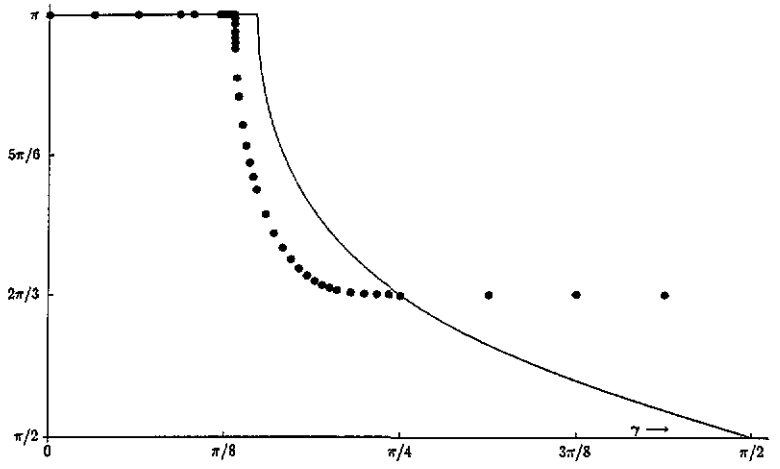

Figure 5. q^* (dots) and θ^* (full line) as functions of γ.

use the truncation error to extrapolate to $n_s = \infty$ and give an estimate of the error which is around 0.01%. At $\tan\gamma = 0.438$ we have $q^* = \pi$ and at $\tan\gamma = 0.4381$ we have $q^*/\pi = 0.9951(1)$ so $\tilde{\gamma}$ lies between these points. $\tilde{C}''(\pi)$, the second moment at $q = \pi$, is very well fitted by a linear function in the region $0.4 < \tan\gamma < 0.5$. Finding the point where the least-squares fit vanishes then yields $\tilde{\gamma} = 0.43806(4)$.

Comparison with the classical model

In the classical analogue of (1.1), the quantum spin operators S_i become classical spin variables which can take on any value on the unit sphere. The energy is

$$E = \sum_i \epsilon(\theta_i) \tag{2.2}$$

where $\epsilon(\theta) = \cos\gamma\cos\theta + \sin\gamma\cos^2\theta$ and θ_i is the angle between S_i and S_{i+1}. This is minimized for

$$\theta_i \equiv \theta^* \tag{2.3}$$

$$= \begin{cases} \pi & 0 \leqslant \gamma \leqslant \tilde{\gamma}_{\mathrm{cl}} \\ \arccos(-(\cot\gamma)/2) & \tilde{\gamma}_{\mathrm{cl}} \leqslant \gamma \leqslant \pi/2 \end{cases} \tag{2.4}$$

where $\tilde{\gamma}_{\mathrm{cl}} \equiv \tan^{-1}\frac{1}{2}$ denotes the position of the onset of the classical spiral phase and θ^* denotes the classical pitch angle.

In the Néel phase $0 \leqslant \gamma \leqslant \tilde{\gamma}_{\mathrm{cl}}$ the classical ground state has the trivial degeneracy of fixing the direction of one of the spins. In the spiral phase $\tilde{\gamma}_{\mathrm{cl}} < \gamma < \pi/2$ the classical ground state has further degeneracy in that the azimuthal angle between successive spins can take on any value. The classical correlation function is obtained by averaging S_iS_j over all classical ground states [22], i.e.

$$C(r) = \tfrac{1}{3}(\cos\theta^*)^r. \tag{2.5}$$

Classically then, $\tilde{C}(q)$ has a quadratic peak at $q = \pi$ in the whole region $0 \leqslant \gamma \leqslant \pi/2$. If, however, we restrict the spiral states so that the S_i lie in a plane and make angle $i\theta^*$ with S_0, then we have $C(r) = \cos(r\theta^*)$ and $\tilde{C}(q)$ has delta function peaks at $q = \theta^*$ and $2\pi - \theta^*$, vanishing elsewhere.

We include a plot of θ^* against γ in figure 5. Clearly, quantum fluctuations break the degeneracy in the classical spiral state, forcing successive spins to lie in a plane. Moreover, the θ^* and q^* curves have marked differences—$\tilde{\gamma} \neq \tilde{\gamma}_{cl}$ and q^* remains fixed at $2\pi/3$ for all $\gamma > \pi/4$. The classical solution is therefore highly unstable against incommensurate distortions of spins. Indeed, equation (1.1) is one of the simplest examples of a quantum model where the $1/S$ expansion away from the classical solution fails [23].

3. Summary and conclusions

We have applied the DMRG to calculate the ground-state correlation function and to define and calculate the periodicity of the ground state of the bilinear–biquadratic spin-1 chain (1.1) in the frustrated regime where both coupling constants are positive.

Combining our study with those of Fáth and Sólyom, we predict that in the region studied (where the quadratic term is antiferromagnetic and the biquadratic term opposes alignment of neighbouring spins) the model has three phases:

(i) $0 \leqslant \gamma \leqslant \tilde{\gamma}$. In this phase the model has short-ranged antiferromagnetic order, $\tilde{C}(q)$ having a quadratic maximum at $q = \pi$ and the ground state having periodicity 2.

(ii) $\tilde{\gamma} < \gamma < \gamma_c$. In this phase the model has short-ranged spiral order, $\tilde{C}(q)$ having a quadratic peak at $q = q^* < \pi$. We define the periodicity of the ground state to be $2\pi/q^*$.

(iii) $\gamma_c \leqslant \gamma < \pi/2$. In this phase the model has quasi-long-range order, $C(r)$ decaying algebraically. The ground state has period 3, $\tilde{C}(q)$ having a cusp singularity at $q = 2\pi/3$.

We estimate $\tan\tilde{\gamma} = 0.438\,06(4)$. The predicition of [17], that $\gamma_c = \pi/4$, is not inconsistent with our results for the peak position q^* and our crude estimates of the correlation length.

Acknowledgments

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