Exact and Numerical Results for a Dimerized Coupled Spin-1/2 Chain

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We establish exact results for coupled spin-1/2 chains for special values of the four-spin interaction V and dimerization parameter δ. The first exact result is at $\delta = 1/2$ and $V = -2$. Because we find a very small but finite gap in this dimerized chain, this can serve as a very strong test case for numerical and approximate analytical techniques. The second result is for the homogeneous chain with $V = -4$ and gives evidence that the system has a spontaneously dimerized ground state. Numerical diagonalization and bosonization techniques indicate that the interplay between dimerization and interaction could result in gapless phases in the regime $0 \leq V < -2$.

The renewed interest in coupled spin-1/2 chains stems from the belief that they are relevant to explain unusual magnetic properties of a wide range of materials. For certain compounds degenerated molecular orbitals may be represented by extra isospin degrees of freedom which are coupled with the true spin through superexchange [1–3]. This analogy has recently been used to propose and study a variety of coupled spin-isospin models with potential experimental relevance [3–5]. Other examples are the so-called spin ladder systems [6]. In this Letter we study the following dimerized coupled spin-1/2 chains:

$$H = J \sum_{i=1}^{L} \sum_{\alpha=1,2} [1 + \delta(-1)^{i+\alpha}] \vec{S}_i^{(\alpha)} \cdot \vec{S}_{i+1}^{(\alpha)}$$
$$+ V \sum_{i=1}^{L} (\vec{S}_i^{(1)} \cdot \vec{S}_{i+1}^{(1)}) \times (\vec{S}_i^{(2)} \cdot \vec{S}_{i+1}^{(2)}), \quad (1)$$

where $\vec{S}_i^{(\alpha)}$, $\alpha = 1, 2$ are two commuting sets of $s = 1/2$ operators (spin and isospin) acting on site i of a lattice of size L. Notice that the dimerization δ is completely staggered, which seems to be the most interesting case at least in the context of spin ladders [7,8]. In spin ladders, the coupling V can be interpreted as a result of the Coulomb interaction between holes in a doped phase [9]. Here, unless stated otherwise, we assume an antiferromagnetic $J > 0$ Heisenberg energy scale.

Much of the theoretical efforts have been focused on the study of the homogeneous chain both numerically [5,10,11] and analytically [12,13]. In general, the interesting features occur in the strong coupling regime where perturbation theory does not work. In these cases it is important to have access to exact results since they can be used as a test case for approximate nonperturbative methods. One such example is the point $V/J = 4$ in the homogeneous chain, which is equivalent to the integrable SU(4) exchange spin chain [14,15]. This fact has been useful not only to check numerical analysis [5,10] but also relevant to trigger further nonperturbative studies [16]. One of the

purposes of this paper is to point out that there exist two other points in which the model (1) is still exactly solvable. Equally important, both results are concerned with the strong coupling regime $|V| \gg J$, namely,

$$\text{(I)} \ \delta = 1/2, \quad V/J = -2,$$
$$\text{(II)} \ \delta = 0, \quad V/J = -4. \quad (2)$$

The exact solution enables us to derive analytical expressions for the ground state energy and the low-lying gap excitation. To our knowledge, the first case is a rare example where we can provide the exact value of the energy gap for an interacting spin chain with *alternating* bond strength. It should be emphasized that this result is both at a feasible value of the spin-Peierls dimerization and in a physically meaningful regime of the coupling V [9]. The utility of these exact results is threefold. First of all, since the lowest gap excitation for case (I) is very small, it provides us a relevant check of the reliability of numerical and approximate nonperturbative methods to distinguish between gapped and gapless phases. Moreover, we present evidence that the second case is an example of a system with a spontaneous spin-Peierls effect. This lends support to the prediction by Nersesyan and Tsvelik [9] that *negative* four-spin interaction can induce non-Haldane spin-liquid behavior in spin ladders. The novelty here is that this fact is established at the very strong coupling regime $V/J = -4$, which is beyond the reach of the approach of Ref. [9]. Finally, together, they motivate us to study the gap behavior for arbitrary values of dimerization and interaction and to search for possible gapless phases.

The exact integrability is derived by identifying the lattice statistical model whose row-to-row transfer matrix commutes with Hamiltonian (1) with the parameters δ and V/J given by (2). Such a classical statistical system consists of two isotropic six vertex models coupled by the total energy-energy interaction. The row-to-row transfer matrix $T(\lambda)$ of a vertex model is usually written as the trace of an

ordered product of Boltzmann weights,

$$T(\lambda) = \mathrm{Tr}_{\mathcal{A}}[\mathcal{L}_{L,\mathcal{A}}^{(1)}(\lambda)\mathcal{L}_{L-1,\mathcal{A}}^{(2)}(\lambda)\cdots\mathcal{L}_{2,\mathcal{A}}^{(1)}(\lambda)\mathcal{L}_{1,\mathcal{A}}^{(2)}(\lambda)],$$
(3)

where $\mathcal{L}_{j,\mathcal{A}}^{(\alpha)}(\lambda)$ denotes the local Boltzmann weights with auxiliary space $\mathcal{A}$ and quantum space $j = 1, \ldots, L$, parametrized by the spectral parameter λ. The auxiliary and quantum spaces correspond to the horizontal and vertical degrees of freedom of the coupled six vertex models together with four possible states per bond.

Essential to our approach is to notice that the Boltzmann weights can be conveniently written in terms of two commuting Temperly-Lieb operators $E_{j,\mathcal{A}}^{(\alpha)} = 2(\vec{S}_j^{(\alpha)} \cdot \vec{S}_A^{(\alpha)} - I_{j,\mathcal{A}}/4)$, where $I_{j,\mathcal{A}}$ is the identity operator. More precisely, defining $\mathcal{L}_{j,\mathcal{A}}^{(\alpha)}(\lambda) = P_{j,\mathcal{A}}R_{j,\mathcal{A}}^{(\alpha)}(\lambda)$ with $P_{j,\mathcal{A}}$ denoting the exchange operator, the R matrix $R_{j,\mathcal{A}}^{(\alpha)}(\lambda)$ is

$$R_{j,\mathcal{A}}^{(\alpha)}(\lambda) = I_{j,\mathcal{A}} + \omega_1(\lambda)E_{j,\mathcal{A}}^{(\alpha)} + \omega_2(\lambda)E_{j,\mathcal{A}}^{(1)}E_{j,\mathcal{A}}^{(2)}.$$ (4)

The weight $\omega_2(\lambda)$ plays the role of the four-spin interaction V while a combination with $\omega_1(\lambda)$ is responsible for the dimerization δ. These weights belong to a more general class of systems that originally appeared in the integrable coupled Potts models [17], and were recently rediscovered in the context of Lorentz lattice gases and Fuss-Catalan algebras [18]. For the cases we are interested in, their explicit expressions are

$$\omega_1(\lambda) = \begin{cases} \frac{e^\lambda - 1}{2} & \text{for I}, \\ 0 & \text{for II}, \end{cases}$$

$$\omega_2(\lambda) = \begin{cases} \frac{e^\lambda(e^\lambda - 1)}{3 - e^\lambda} & \text{for I}, \\ \frac{\sinh(\lambda)}{\sinh(\gamma - \lambda)} & \text{for II}, \end{cases}$$
(5)

where $\gamma = \ln(2 + \sqrt{3})$.

As usual, the corresponding Hamiltonian is obtained as the first-order expansion in λ of the logarithm of $T(\lambda)$. By using the weights (5) it is not difficult to verify that we indeed recover the Hamiltonian (1), up to irrelevant rescaling constants, at the values given by (2). To make further progress we have to explore other properties of the transfer matrix. In particular, we are interested in establishing the inversion relation [19–21], since it provides us the means to compute the ground state energy and excitation properties. We will start by considering the most involved model which is the case with non-null dimerization $\delta = 1/2$. Even though the Bethe ansatz solution of this model has eluded us so far, the inversion relation is sufficient to provide us exact results for relevant quantities such as the gap. For this system, the inversion identity follows from a combination between the usual unitary property, $\mathcal{L}_{1,2}^{(\alpha)}(\lambda)\mathcal{L}_{2,1}^{(\alpha)}(-\lambda) = I_{1,2}$, and a less standard crossing relation for the weights $\mathcal{L}_{1,2}^{(\alpha)}(\lambda)$. While these operators are

not separately crossing symmetric, they do satisfy a novel "mixed" crossing property, which reads

$$\mathcal{L}_{1,2}^{(\alpha)}(\lambda) = \frac{\omega_1(\lambda)}{\omega_1(\ln3 - \lambda)} \overset{1}{M}[\mathcal{L}_{1,2}^{(3-\alpha)}]^{t_2}(\ln3 - \lambda)\overset{1}{M},$$ (6)

where t_k denotes the transpose and $\overset{k}{M}$ is a 4×4 antidiagonal matrix both acting on the space k. Together with unitarity, this crossing relation allows us to derive the following inversion identity:

$$T^{(\mathrm{I})}(\lambda)T^{(\mathrm{I})}(\lambda + \ln3) = \left[\frac{\omega_1(\ln3 + \lambda)}{\omega_1(-\lambda)}\right]^L \mathrm{Id} + T^+(\lambda),$$
(7)

where $T^+(\lambda)$ is a matrix whose elements for large L are exponentially small and Id is the identity. This means that, in the thermodynamic limit, the last term in (7) vanishes, providing us a much simpler functional equation for all the transfer matrix eigenvalues. In particular, the largest eigenvalue $\Lambda_{\mathrm{gs}}^{(\mathrm{I})}(\lambda)$ per site satisfies

$$\Lambda_{\mathrm{gs}}^{(\mathrm{I})}(\lambda)\Lambda_{\mathrm{gs}}^{(\mathrm{I})}(\ln3 + \lambda) = \frac{\omega_1(\ln3 + \lambda)}{\omega_1(-\lambda)}.$$ (8)

With the help of unitarity, $\Lambda_{\mathrm{gs}}^{(\mathrm{I})}(\lambda)\Lambda_{\mathrm{gs}}^{(\mathrm{I})}(-\lambda) = 1$, it is possible to solve the functional equation (8) under a plausible analyticity assumption in the region $0 \leq \lambda < \ln3$ (positive Boltzmann weights). The solution is

$$\Lambda_{\mathrm{gs}}^{(\mathrm{I})}(\lambda) = (e^\lambda - 1)\prod_{j=0}^{\infty} \frac{(e^\lambda 3^{2j+1} - 1)}{(e^\lambda 3^{2j} - 1)} \frac{(e^{-\lambda}3^{2j+2} - 1)}{(e^{-\lambda}3^{2j+1} - 1)}$$
(9)

which allows us to derive the exact value for the ground state energy per site $E_{\mathrm{gs}}^{(\mathrm{I})}/J$ of Hamiltonian (1) at $\delta = 1/2$ and $V/J = -2$. This value is obtained by computing $E_{\mathrm{gs}}^{(\mathrm{I})}/J = -\frac{d \ln\Lambda_{\mathrm{gs}}^{(\mathrm{I})}(\lambda)}{d\lambda}|_{\lambda=0} + 3/8$, which reads

$$E_{\mathrm{gs}}^{(\mathrm{I})}/J = -\frac{5}{8} - 12\sum_{j=0}^{\infty} \frac{3^{2j}}{(3^{2j+1} - 1)(3^{2j+2} - 1)}.$$ (10)

The inversion relation and trigonometric periodicity impose stringent constraints on the form of the low-lying excitations. They should be described in terms of meromorphic functions having two independent periods $2\ln(3)$ and $2\pi i$. This observation alone enables us to calculate the dispersion relation [21] and from that one obtains the exact value for the gap. Such a gap corresponds to the energy necessary to create an excitation with total spin $S^z = 1$. Here we omit further technicalities and the result for the triplet energy gap $\Delta^{(\mathrm{I})}/J$ is

$$\frac{\Delta^{(\mathrm{I})}}{J} = \prod_{j=1}^{\infty}\left[\frac{(1 - 3^{-j/2})}{(1 + 3^{-j/2})}\right]^2 = 0.002\,869\,614.$$ (11)

Interesting enough, the energy gap is very small and this has an immediate application. It could be used to test if a given numerical or approximate nonperturbative method can really make a clear distinction between a small gap and a real gapless phase. In general, this is a difficult task, and we expect that our exact result will be quite relevant

to determine suitability of multiprecision methods in spin ladder models. This should be important when one wants to predict the scaling behavior of the gap as a function of the dimerization [22].

We turn next to the second solvable point $\delta = 0$ and $V/J = -4$. In this case, $\omega_1(\lambda)$ is null and we are left only with the product of two commuting isotropic six vertex models. From the point of view of the classical statistical model, this means that we are in fact dealing with an alternative representation of the sixteen-state Potts model. By now several properties of the general q-state Potts are fairly well understood. In particular, the ground state and the triplet gap can be determined either by the inversion trick as above [21] or by a direct mapping onto the XXZ Heisenberg chain [23] and they are given by

$$\frac{E_{gs}^{(II)}}{J} = -\sqrt{3}\left[1 + 4\sum_{j=1}^{\infty} \frac{1}{1+(2+\sqrt{3})^{2j}}\right] + \frac{1}{4}, \quad (12)$$

and

$$\frac{\Delta^{(II)}}{J} = 2\sqrt{3}\prod_{j=1}^{\infty}\left[\frac{[1-(2+\sqrt{3})^{-j}]}{[1+(2+\sqrt{3})^{-j}]}\right]^2 = 0.779\,604\,542. \quad (13)$$

Further interesting results can still be derived from the mapping of the homogeneous model (1) at $V/J = -4$ onto the antiferromagnetic XXZ chain with anisotropy $J^z/J^x = 2$ [21,23]. First, it is possible to show that the gap of the first excitation in the sector of total spin $S^z = 0$ vanishes exponentially as $L \to \infty$. The momentum of this excitation is π, which leads to the conclusion that in the thermodynamic limit the system has two spontaneously dimerized ground states, in accordance with the Lieb-Schultz-Mattis theorem [24,25]. This result supports the prediction by Nersesyan and Tsvelik [9] that a four-spin interaction may induce dimerized phases in spin ladder models. The bosonization arguments of Ref. [9] for the weak coupling regime $|V|/J \ll 1$ together with our exact result at the very strong coupling point $V/J = -4$ indicate that such dimerized phase should be robust for a rather large region of $V < 0$. Next, one can explain the numerical observations by Pati, Singh, and Khomskii [5] that the model (II), *now for $J < 0$*, possesses an infinitely

degenerated ground state. In fact, $J < 0$ corresponds to the *ferromagnetic* regime of the XXZ chain, whose $T = 0$ finite entropy for $J^z/J^x = -2$ is exactly computed to be $\ln(2 + \sqrt{3})$. This value is a rigorous confirmation of the lower bound proposed in Ref. [5] for such residual entropy.

Considering these exact results, it is natural to ask if a combined effect of dimerization and *negative* four-spin interaction could lead to a gapless regime. To investigate this problem we numerically diagonalize the Hamiltonian (1), with periodic boundary conditions, up to $L = 14$ sites by using a Lanczos-type algorithm. In Table I we exhibit our numerical results for the ground state energy and the triplet energy gap for both cases (I) and (II). The extrapolations towards the infinite volume limit were performed by using the Van den Broeck–Schwartz method of convergence [26]. While the results for the ground state are in good agreement with the exact values, the gap estimates have a rather poor accuracy. This emphasizes the importance of our exact results, specially for model (I), since they clearly show that one cannot trust the numerical gap estimates beyond two significant digits. However, we can still make a *qualitative* comparison of the behavior of the gap in the whole dimerization region $0 \leq \delta \leq 1$ for various values of the interaction V.

This is illustrated in Fig. 1 for three values of V in the strong coupling regime. We observe that indeed for each value of V/J the gap has a very small minimum for an appropriate value of the parameter δ. Note that for $V/J = -2$ this minimum occurs very near the solvable point $\delta = 1/2$ where the gap is small but still finite. This helps us to establish an upper bound for V/J, beyond which one probably should rule out strictly null mass gaps. For $V/J < -2$ we observe, however, that this minimum decreases faster towards zero, suggesting the possibility of a gapless line on the plane $(\delta, V/J)$ in the $0 \leq V/J < -2$ regime. To provide an independent check of this possibility we have analyzed the continuum limit of Hamiltonian (1) by bosonization techniques [8,9]. For weak couplings this analysis predicts a massless excitation on the critical line $|V|/J \sim \delta^2$ which is in accordance with our numerical results up to an accuracy of two digits. Though these are strong evidence of the existence of a massless line it is still interesting to confirm this finding through more powerful

TABLE I. Finite size and extrapolated results for the ground state energy and the triplet gap for cases (I) and (II). For comparison we also exhibit the exact results.

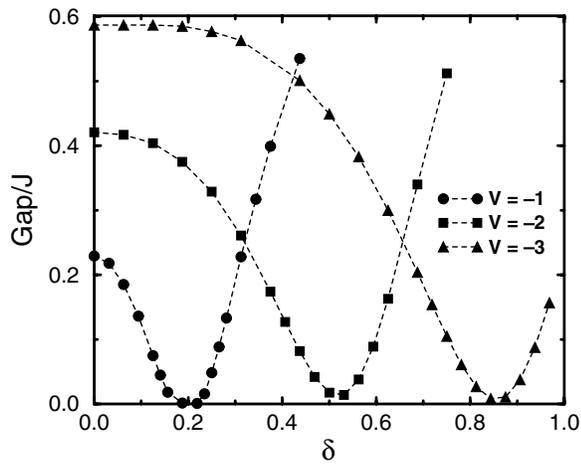| L	$E_{gs}^{(I)}/J$	$E_{gs}^{(II)}/J$	$\Delta^{(I)}/J$	$\Delta^{(II)}/J$
4	-1.625	-2.25	2.267 949	4.0
6	$-1.510\,455$	$-2.083\,333$	1.529 642	2.876 894
8	$-1.474\,743$	$-2.033\,159$	1.162 347	2.306 000
10	$-1.459\,071$	$-2.012\,015$	0.939 894	1.957 187
12	$-1.450\,822$	$-2.001\,389$	0.790 102	1.722 250
14	$-1.445\,954$	$-1.995\,437$	0.682 160	1.553 984
Extrap.	$-1.4331\,(\pm 1)$	$-1.983\,(\pm 1)$	0.011 (± 3)	0.744 (± 2)
Exact	$-1.433\,126$	$-1.984\,444$	0.002 869	0.779 604

FIG. 1. Extrapolated triplet energy gap Δ/J for $V/J = -1$, -2, and -3. For $V/J \leq -4$ we no longer observed a local minimum for the gap in the interval $0 \leq \delta \leq 1$.

numerical methods such as the density matrix renormalization group [27]. In particular, because this method could provide good accuracy on the critical value V/J where the gapless line starts and its performance can readily be tested by using the exact gap value of case (I). In practice, however, when a gap is as small as we calculated, its effect would be invisible at even low temperatures which may still be considerably higher than the value of the gap.

In summary, we have pointed out the existence of two integrable points in coupled spin-$1/2$ chains where relevant physical quantities such as the ground state energy and the excitation gap can be evaluated exactly. These results together with the solvable SU(4) symmetric point seem to exhaust all possible Bethe ansatz integrable cases of Hamiltonian (1). In addition, numerical and bosonization analyses indicate the possibility of a gapless line on the plane $(\delta, V/J)$ for $0 \leq V/J < -2$. This then will add another example of coupled spin chains in which a suitable combination of dimerization and interaction strength is capable to close the energy gap [7,8]. We also hope that our observations will motivate further numerical and analytical investigation in related systems.

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