Effects of a space modulation on the behavior of a 1D alternating Heisenberg spin-1/2 model

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Abstract
The effects of a magnetic field ($h$) and a space modulation ($\delta$) on the magnetic properties of a one-dimensional antiferromagnetic–ferromagnetic Heisenberg spin-1/2 model have been studied by means of numerical exact diagonalization of finite size systems, the nonlinear $\sigma$ model, and a bosonization approach. The space modulation is considered on the antiferromagnetic couplings. At $\delta = 0$, the model is mapped to a gapless Lüttinger liquid phase by increasing the magnetic field. However, the space modulation induces a new gap in the spectrum of the system and the system experiences different quantum phases which are separated by four critical fields. By opening the new gap, a magnetization plateau appears at $\frac{1}{2}M_{\text{sat}}$. The effects of the space modulation are reflected in the emergence of a plateau in other physical functions such as the F-dimer and the bond-dimer order parameters, and the pair-wise entanglement.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
The effects of a magnetic field on the magnetic properties of low-dimensional quantum magnets at zero temperature have attracted much attention in recent years. One of the very interesting phenomena is the appearance of a magnetization plateau in the magnetization curve. This behavior can be viewed as an essentially macroscopic quantum phenomena, and has gained much attention recently. When a plateau appears the energy gap is opened, which can in some senses be regarded as a kind of generation of the Haldane conjecture [1]. In a seminal work, Oshikawa, Yamanaka, and Affleck studied the magnetization of a general class of Heisenberg spin chains in the presence of a magnetic field. They showed that the plateaus can appear when the magnetization per site $m$ is topologically quantized by $n(s - m) = \text{integer}$, where $s$ is the magnitude of the spin, and $n$ is the period of the ground state determined by the explicit spatial structure of the Hamiltonian [2].

The bond alternating Heisenberg spin-1/2 chains which are obtained by a space modulation in the exchange couplings [3–9] are a particular class of the low-dimensional quantum magnets to observe the magnetization plateau at zero temperature. The bond alternating antiferromagnetic–ferromagnetic spin-1/2 chains have a gap in the spin excitation spectrum and reveal extremely rich quantum behaviors in the presence of an external magnetic field [10–13]. By tuning the magnetic field, the excitation gap is reduced and reaches zero at the first critical field. Simultaneously, the magnetization starts to increase up to its saturation value, 0.5, at the second critical field. More enhancement of the field reopens the gap and the saturation plateau appears in the magnetization curve. These models have only two plateaus at zero and saturation values of the magnetization. It has been found that a space modulation in the exchange couplings can affect the behavior of the field induced magnetization. For
example the bond alternating ferromagnetic–ferromagnetic–antiferromagnetic (F–F–AF) trimerized Heisenberg spin-1/2 chains have exotic behaviors by changing the magnetic field [14]. This model can be realized in Cu compounds such as 3CuCl2·2dx. The magnetization has a plateau at \( \frac{M}{M_{\text{sat}}} = \frac{1}{3} \), where \( M \) and \( M_{\text{sat}} \) are the magnetization and its saturated values, respectively [15, 16]. The mid-plateaus have also appeared in the bond alternating ferromagnetic–antiferromagnetic–antiferromagnetic (F–AF–AF) trimerized Heisenberg spin-1/2 chains [17]. It has also been shown that the static structure factor does not vary with the external magnetic field at the plateau state [18].

The other examples are the tetrameric bond alternating ferromagnetic–ferromagnetic–antiferromagnetic–antiferromagnetic (F–F–AF–AF) Heisenberg spin models. A realization for the spin-1 model has been shown in figure 1. The bond alternating ferromagnetic–antiferromagnetic–antiferromagnetic (F–AF–AF) trimerized Heisenberg spin-1/2 chains [17]. It has also been shown that the easy way to obtain the effective model, which manifestly displays a mechanism for the generation of the sequence of new scales, is to start from the limit of a noninteracting block of pairs \( J_F = 0 \) and strong magnetic field \( h \approx J_{AF} \) [24]. In the limiting case of strong AF coupling \( J_{AF} \gg J_F \) and \( J_{AF} \gg \delta J_{AF} \) the model can be mapped to an effective spin chain Hamiltonian [12]. At \( J_{AF} \gg J_F \), the system behaves as a nearly independent block of pairs. Indeed, an individual block of spin pairs may be in a singlet or a triplet state with the corresponding eigenvalues given by

\[
E^\pm(T) = \frac{1}{2} J_{\text{AF}}^\pm - h,
\]

\[
E^\pm(T_0) = \frac{1}{2} J_{\text{AF}}^\pm + h.
\]  

When \( h \) is small, the ground state consists of a product of pair singlets. As the magnetic field \( h \) increases the energy of the triplet state \( |T_1\rangle \) decreases and at \( h = J_{\text{AF}}^+ \) forms together with the singlet state, a doublet of almost degenerate low energy states, split from the remaining high energy two triplet states. Thus, for a strong enough magnetic field we have a situation when the singlet \( |S\rangle \) and triplet \( |T_1\rangle \) states create a new effective spin \( \tau = 1/2 \) system. On the new singlet–triplet subspace and up to a constant, we easily obtain the effective Hamiltonian

\[
H^\text{eff} = -\frac{J_F}{2} \sum_{j=1}^{N/2} \left[ \tau_j^+ \tau_{j+1}^- + \tau_j^- \tau_{j+1}^+ + \frac{1}{2} \tau_j^x \tau_{j+1}^x \right] - h^\text{eff} \sum_{j=1}^{N/2} \left( -1 \right)^j \tau_j^z,
\]  

where \( h^\text{eff} = h - J_{\text{AF}} + \frac{J_F}{2} \) and \( h^\text{eff} = \delta J_{\text{AF}} \). The effective Hamiltonian is nothing but the XXZ Heisenberg chain, with anisotropy \( \Delta = 1/2 \) in a uniform and staggered longitudinal magnetic field. The full phase diagram of this model has been investigated by Alcaraz and Malvezzi [25] and the nature of the ground state phase transition has been pointed out in [26]. The other properties can be found in recent works such as [2, 27–29]. To find a clearer picture for the low energy spectrum of the effective model (3), using the numerical Lanczos method, we have computed the energy gap of the

Figure 1. Schematic representation of a tetrameric spin chain.
3. Field theory predictions

In this section we will study the model (1) in the language of two continuum field theories. We have employed the nonlinear $\sigma$ model and bosonization approaches to obtain the energy gap, the critical fields, and magnetization plateaus of the model.

3.1. Nonlinear $\sigma$ model

The O(3) nonlinear $\sigma$ model (NL$\sigma$M) is a semiclassical approach which is based on certain properties of a field theory in $(1+1)$ dimensions. In 1983 Haldane predicted theoretically the existence of a finite gap between the ground state and the first excited state of antiferromagnetic Heisenberg integer spin chains [1]. He also conjectured that the half-odd integer spin chains are gapless. The Hamiltonian of a homogeneous spin chain is mapped to an O(3) NL$\sigma$M with an additional topological term. The topological term is 0 if spins of the chain are integer and $\pi$ if they are half-odd integer.

In the following we will investigate the low temperature behaviors of the alternating spin chain (1). For convenience in the calculations, let us write the Hamiltonian (1) in the following form:

$$H = -J_F \sum_{j=1}^{N/4} \left( S_{2j-1}^{(1)} \cdot S_{2j}^{(2)} + S_{2j-1}^{(1)} \cdot S_{2j}^{(2)} \right) + J_{AF} \sum_j \left[ \left(1 + \delta \right) S_{2j}^{(2)} \cdot S_{2j+1}^{(1)} \right] + \hbar \sum_j S_j^z,$$

where $0 \leq \delta \leq 1$. Using the spin coherent states representation for the spin operators, i.e. $S = \sigma \Omega$, we can write the Hamiltonian in terms of the classical spin vectors. By introducing three classical fields $n$, $L$, and $\Delta$ the classical vectors are written in the following forms:

$$\Omega_{2j-1}^{(i)} = -n_{2j-1} \left( 1 - \left( \frac{a}{s} \right)^2 L_{2j-1} \right)^{1/2} + \frac{a}{s} L_{2j-1},$$

$$\Delta_{2j} = \frac{(-1)^j a}{s} \Delta_{2j-1},$$

where $i = 1, 2$ and $\sigma$ is the lattice constant. Typically, for a quantum antiferromagnetic Heisenberg chain it is convenient to write the spin vectors in terms of a unimodular Néel field ($n$) and one ferromagnetic canting field ($L$). However, for an alternating AF–F Heisenberg spin chain, the main difficulty arises from the fact that it is inhomogeneous and writing a continuous action out of the discrete Hamiltonian is not a trivial task [30]. Using another field which describes the variation of the Néel fields inside the two spin-blocks such as $\Delta$ we can map the Hamiltonian (4) to the following O(3) NL$\sigma$M:

$$\frac{1}{2g} \int_0^{L} \int_0^L dx \, d\chi \, \left[ (\partial_\chi n) + (\partial_{\chi x} n) \right]^2 - i \Theta W,$$

where $W$ is the winding number, $L_T = c\beta$, $x_0 = ct$, and we have considered the case $h = 0$. By defining $\alpha = \frac{J_{AF}}{J_F}$, the coupling constant $g$ and the velocity of spin excitations $c$ are given in terms of $\alpha$ and $\delta$ as

$$g = \frac{1 - \delta}{s \left( 1 + \frac{\delta}{4} \right)} \left[ 1 + \frac{\delta}{s} \left( 1 + \frac{\delta}{2(1 + \alpha)} \right) \right]^{1/2},$$

$$c = J_{AF} \alpha s \left( 1 - \frac{\delta^2}{4} - \frac{1}{2(1 + \alpha)} \right)^{1/2}.$$

The topological $\Theta$ term is obtained as follows:

$$\Theta = 2\pi \left( \frac{s \delta \alpha}{1 + \alpha - \frac{\delta}{2}} \right).$$
where for $\alpha = 0$ or $\delta = 0$ the topological $\Theta$ term is zero and the model is always gapped and the spin excitation velocity is $\frac{1}{c} J_{eff}sls$. Moreover, the $\alpha = 1$ and $\delta = 0$ is the special case of AF–F Heisenberg spin chains in which the topological term is always $0$. This result is in good agreement with the result presented in [30]. For any other values of $\alpha$ and $\delta$, the Hamiltonian is mapped to the following NL $\sigma M$ with $\Theta$ in the interval $[0, \pi]$. This model is also gapped and the gap value is dependent on $\alpha$ and $\delta$.

Now, let us study the model in the presence of the magnetic field. Since, the model is always gapped in the absence of a magnetic field we are allowed to consider $\Theta = 0$. The Hamiltonian (4) is mapped to the following NL $\sigma M$ in which the effect of the magnetic field is clearly seen:

$$ A = \frac{1}{2g} \int d^2x \left( (\partial_x n)^2 + \left( \frac{i}{c} h \times n \right)^2 \right). \quad (9) $$

To obtain more physical insight from the effects of the magnetic field, it may be more physically transparent to work with two fields $(\theta, \phi)$ where $n = (\sin \theta \sin \phi, \sin \theta \cos \phi, \cos \theta)$. Here $\theta$ is co-latitude and $\phi$ is azimuthal angle. Selecting magnetic field in the $z$ direction, the action (9) takes the following form:

$$ A = \frac{1}{2g} \int d^2x \left\{ (\partial_n \theta)^2 + \sin^2 \theta \left[ (\phi')^2 + \frac{1}{c^2} (\phi - ih)^2 \right] \right\}, \quad (10) $$

where $\theta$ is the angle of $h$ and $n$. In the term, $h \times n$, the magnetic field induces a hard-axis anisotropy. In other words, the magnetic field tries to align all spins with $n$ in the plane normal to $h$. Thus for the high field regime, $h > |\phi|$, the deviation of Néel field $n$ from the plane is small. Thus an expansion to quadratic order in $\theta$ is valid. The action is

$$ A = \frac{1}{2g} \int d^2x \int_0^L dt \left\{ (\partial_n \theta)^2 - \theta^2 \left[ (\partial_n \phi)^2 - \frac{2h}{c} \partial_n \phi \right] \right\}, \quad (11) $$

where $h = h/c$ and the fluctuations have been separated to the in-plane and out-of-plane fluctuations.

Using a spin stiffness analysis, $1/N$ expansion and a renormalization group approach, the magnetization and spin correlation functions of a spin ladder in an applied magnetic field [31, 32] have already been computed. The magnetization $(\sum_i \frac{S_i^z}{N})$ is given by $M = \frac{1}{N} S_0^z$ where $F = -\frac{2}{\beta} \ln Z$ is the Helmholtz free energy and $Z = \int F \partial \phi \partial \phi^\dagger e^{-F}$. The separable nature of fluctuations allows us to give the results of $M = M_0 + M_1$, which is a summation of both out-of-plane and in-plane contributions. At low enough temperatures and small value of $c/h$ one can find that the out-of-plane contribution is a constant, $M_0 = 1/2$, which corresponds to a uniform state. The in-plane contribution has two terms, one is linear in the field and the other has a sawtooth form (see [32]). In total, $M_1$ has a step-like form in which the width of the steps scales as $1/N$. Thus the sawtooth form is the finite size correction and in the thermodynamic limit $N \rightarrow \infty$ the in-plane magnetization is only linear.

For our tetramerized spin chain the magnetization is given by

$$ M \simeq -1 + \frac{h}{g c}. \quad (12) $$

Application of a high enough magnetic field will cause spin alignment, or saturation with a maximum magnetization, $M_s = s$. This effect should be considered in the NL $\sigma M$ approach by a Lagrange multiplier. At zero magnetic field the system is gapped and the magnetization is zero. Tuning the magnetic field decreases the gap until the first critical field, $h_{c1}$, where magnetization starts to increase. At the second critical field, where the magnetization is saturated, the gap reopens and spins are fully aligned in the magnetic field direction.

The critical fields which are attained by means of NL $\sigma M$ are as follows:

$$ h_{c1} = gc, \quad h_{c2} = \frac{3}{2} gc. \quad (13) $$

3.2. Bosonization

In this section we concentrate our attention on the low energy and long wavelength excitations by using bosonization language. Let us consider the Hamiltonian (3). In our analysis of the model (3) we closely follow the route developed in the [27]. In the absence of both magnetic fields, $h_0^{eff} = 0$ and $h_1^{eff} = 0$, we have the XXZ spin-1/2 chain with F coupling and anisotropy parameter $\Delta = 1/2$. This model is critical and the long wavelength excitations are described by the following Gaussian theory:

$$ H = \frac{v}{2} \int dx \left\{ (\partial_x \phi)^2 + (\partial_y \phi)^2 \right\}, \quad (14) $$

where $\phi(x)$ and $\phi(x)$ are dual bosonic fields, $\partial_i \phi = \partial_i \phi$, and satisfy the following commutation relations:

$$ [\phi(x), \theta(y)] = i \theta(y - x), \quad (15) $$

$$ [\phi(x), \theta(x)] = \frac{1}{2}. \quad (16) $$

$v$ is the spin excitation’s velocity and is fixed by the Bethe ansatz solution as

$$ v = \left( \frac{J_0}{2} \right) \frac{K}{2K - 1} \sin \left( \frac{\pi}{2K} \right), \quad (17) $$

where the Lütttinger parameter $K$ (the inverse of a boson’s radius [33]) is given as a function of $\Delta$ as

$$ K = \frac{\pi}{2 \arcsin \Delta}. \quad (18) $$

Thus $K$ increases monotonically along the XXZ critical line $-1 < \Delta < 1$ from its minimal value $K = 1/2$ (for the isotropic AF $\Delta = 1$ case) to unity at $\Delta = 0$ (for the noninteracting case) and goes to infinity at $\Delta = 1$ which is the F instability point. Meanwhile the boson radius has its maximum value $(2\pi)^{-1/2}$ for the isotropic AF chains and decreases by changing in $\Delta$ and goes to zero at the F instability point.
The maximum value of the spin excitation velocity occurs where $K \sim 1/2$ or $\Delta = -1$. It decreases monotonically by increasing $K$ and reaches the zero value at $K = \infty (\Delta = 1)$. The continuum limit of the Hamiltonian (3) is obtained by writing spin operators in terms of bosonic fields:

$$
\tau_{\pm}^a = \frac{1}{\sqrt{2\pi}} e^{\pm i\sqrt{\pi} \tau(x)} ( (-1)^a b \sin[\sqrt{4\pi K} \phi(x)] + c) ,
$$

where $a$, $b$, and $c$ are non-universal real constants of the order of unity and they depend on the parameter $\Delta$ [34, 35]. In the above transformations we have made the rotations $\tau_{\pm}^a \rightarrow (-1)^a \tau_{\pm}^a$ and $\tau_{\pm}^a \rightarrow \tau_{\pm}^a$ on the standard bosonic version of the spin operators, as found extensively in the literature. Using (19), the effective Hamiltonian density is given as

$$
\mathcal{H} = \frac{\nu}{2} \left[ (\partial_\theta \phi)^2 + (\partial_\phi \phi)^2 \right] + \frac{\hbar_{\text{eff}}^2}{\pi a_0} \sin[\sqrt{4\pi K} \phi] - \hbar_{\text{eff}} \sqrt{K} \pi \partial_\phi.
$$

The mapped model is nothing but the massive sine-Gordon (SG) model with an additional topological term. Let us first consider the SG model without the topological term $\hbar_{\text{eff}}^2 = 0$ or at the magnetic field value $h = J_{\text{AF}} - \frac{K}{2}$. As has been discussed in many places, in the interval $1 < K < 2$ the spectrum of the SG model contains a soliton and anti-soliton with mass $M$. The exact relation between the soliton mass and the bare mass $\hbar_{\text{eff}}^2$ is as follows [36]:

$$
M = C(K) \hbar_{\text{eff}} \sqrt{\pi},
$$

$$
C(K) = \frac{2\Gamma\left(\frac{3}{4}\right)}{\sqrt{\pi} \Gamma\left(\frac{1}{4} + \frac{\pi}{2}\right)} \left[ \frac{\Gamma\left(1 - \frac{\pi}{4}\right)}{2 \Gamma\left(\frac{3}{4}\right)} \right]^{\frac{1}{4}}.
$$

By substituting $K = 3/2$ and $\hbar_{\text{eff}}^2 = \delta J_{\text{AF}}$ in (21) the soliton mass or equivalently the excitation gap is given as $M \sim \frac{1}{2\sqrt{\pi}} (\delta J_{\text{AF}})^{3/2}$. Tuning $\hbar_{\text{eff}}^2$ adds a gradient term to the gapped SG model. This term creates a shift in the field $\phi$. Actually, in the absence of the topological term the excitation spectrum of the model is gapped and the field $\phi$ is stuck on one of the minima where $(\sin \sqrt{4\pi K}) = -1$. This corresponds to a staggered AF order in the effective spin chain. Tuning the uniform field $\hbar_{\text{eff}}^2$, the number of particles is decreased and the minimum is shifted. A challenge between the two uniform and staggered fields causes the system to experience a different phase when $|\hbar_{\text{eff}}^2| > M$ [37]. This phase transition occurs at $h_c^\pm$ where the excitation gap has reopened.

Consequently the width of the magnetization plateau is obtained as

$$
h_{\text{c1}}^+ - h_{\text{c2}}^- \simeq \frac{4}{J_F} (\delta J_{\text{AF}})^3 ,
$$

where $h_{\text{c1}}^+$ and $h_{\text{c2}}^-$ are the middle critical field and are given by

$$
h_{\text{c1}}^+ = J_{\text{AF}} \left( 1 + \frac{\alpha^2}{4} \right) .
$$

Summarizing, implementing two continuum field theories we found that the model has four critical fields.

**Figure 3.** Difference between the two lowest energy levels of the original Hamiltonian versus the magnetic field $h$ for chains with different lengths $N = 16, 20$ and exchange parameters $J_F = 1.0$, $J_{\text{AF}} = 9/2$, and $\delta = 1/9$.

### 4. Numerical results

To explore the nature of the spectrum and the quantum phase transition, we have used the Lanczos method to diagonalize numerically chains with length up to $N = 28$.

First, we have computed the three lowest energy eigenvalues of chains with $J_F = 1.0$, different values of the length and AF exchanges. To get the energies of the few lowest eigenstates we consider chains with periodic boundary conditions.

In figure 3, we present the results of these calculations for the exchange $J_F = 1.0$, $J_{\text{AF}} = 9/2, \delta = 1/9$, and chain sizes $N = 16, 20$. We define the excitation gap as a gap on the first excited state. As seen in figure 3, in the strong limit of AF exchange, this difference is characterized by the indistinguishable (within the used numerical accuracy) dependence on the chain length and shows a universal linear decrease with increasing magnetic field. At $h = 0$ the spectrum of the model is gapped. Tuning the magnetic field the energy gap decreases linearly with $h$ and vanishes at $h_{\text{c1}}$. This is the first level crossing between the ground state energy and the first excited state energy. The spectrum remains gapless for $h_{\text{c1}} < h < h_{\text{c2}}^-$, whereas the gap is reopened when $h > h_{\text{c2}}^+$. After an increase and a decrease the spin gap goes to zero and vanishes at $h_{\text{c2}}^+$. On further increasing the field $h > h_{\text{c2}}^+$, the spectrum remains gapless up to the critical saturation field $h_{\text{c3}}$. Finally, at $h > h_{\text{c3}}$ the gap is reopened and for a sufficiently large field becomes proportional to $h$. Oscillations of the energy gap in regions $h_{\text{c1}} < h < h_{\text{c2}}^-$ and $h_{\text{c2}}^- < h < h_{\text{c3}}^-$ are the result of level crossings in finite size systems. To find the critical fields we have used the phenomenological renormalization group (PRG) method [12]. The critical field values are given as follows:

$$
\begin{align*}
\delta h_{\text{c1}} = 3.80 \pm 0.01, & \quad h_{\text{c2}} = 4.71 \pm 0.01, \\
\delta h_{\text{c2}} = 3.99 \pm 0.01, & \quad h_{\text{c3}} = 4.58 \pm 0.01.
\end{align*}
$$

\[5\]
To study the magnetic order of the ground state of the system, we start with the magnetization process. First, we have implemented the Lanczos algorithm on finite chains to calculate the lowest eigenstate. The magnetization along the field axis is defined as

$$M^z = \frac{1}{N} \sum_{j=1}^{N} \langle \text{GS} | S_j^z | \text{GS} \rangle,$$  \hspace{1cm} (25)$$

where the notation $\langle \text{GS} | \cdots | \text{GS} \rangle$ represents the ground state expectation value. In figure 4, we have plotted $M^z$ as a function of the magnetic field $h$, and for a chain with exchange parameters $J_F = 1.0$, $J_{AF} = 9/2$, $\delta = 1/9$, and different lengths $N = 20, 24, 28$. As is clearly seen in figure 4 besides the standard singlet and saturation plateaus at $h < h_c^-$ and $h > h_c^+$ respectively, we observe a plateau at $M = \frac{1}{2} M_{\text{sat}}$. Observed oscillations of the magnetization at $h_{c_0} < h < h_c^-$ and $h_c^+ < h < h_c$ result from the level crossing between the ground and the first excited states of this model in the gapless phases. To check that the mid-plateau is not a finite size effect, we performed size scaling [38] of its width and gapless phases. To check that the mid-plateau is not a finite size effect, we performed size scaling [38] of its width and gapless phases. To check that the mid-plateau is not a finite size effect, we performed size scaling [38] of its width and gapless phases.

In particular, we calculated the string correlation function for different finite chain lengths. Since the present model has a $SU(2)$ symmetry in the absence of a magnetic field, we only consider the $z$ component of the string correlation function. In figure 5, we have plotted $O_{\text{S0}}(l, N)$ as a function of $h$ for the chain with exchanges $J_F = 1.0$, $J_{AF} = 9/2$, $\delta = 1/9$ and lengths $N = 20, 24, 28$. As can be seen from this figure, at $h < h_{c_0}$, the string correlation function $O_{\text{S0}}(l, N)$ is saturated and the tetrameric chain system is in the Haldane phase. The Haldane phase remains stable even in the presence of a magnetic field less than $h_{c_1}$.

An additional insight into the nature of different phases can be obtained by studying the correlation functions. We define the following weak and strong bond dimerization order parameters;

$$d_r^w = \frac{4}{N} \sum_{j=1}^{N/2} \langle \text{GS} | S_{2j-1} \cdot S_{2j} | \text{GS} \rangle,$$  \hspace{1cm} (26)$$

$$d_r^s = \frac{4}{N} \sum_{j=1}^{N/2} \langle \text{GS} | S_{2j-1} \cdot S_{2j} | \text{GS} \rangle,$$  \hspace{1cm} (27)$$

where summations are taken over the weak and strong AF bonds. In figure 6 we have plotted $d_r^w$ and $d_r^s$ versus magnetic
field $h$ for chains of lengths $N = 20, 24, 28$ with the exchange parameters $J_{F} = 1.0, J_{AF} = 9/2$, and $\delta = 1/9$. As seen from this figure, at $h < h_{c1}$, spins on all AF bonds are in a singlet state $d_{s}^{w} = d_{s}^{c} \simeq -0.75$, while at $h > h_{c2}$, $d_{s}$ is equal to the saturation value $d_{s}^{w} d_{s}^{c} \sim 1/4$ and F long-range order along the field axis is present. However, in the considered case of strong AF exchanges ($J_{AF} \gg J_{F}$) and high critical fields, quantum fluctuations are substantially suppressed and calculated averages of on-AF-bond spin correlations are very close to their nominal values.

On the other hand, for intermediate values of the magnetic field, at $h_{c1} < h < h_{c2}$, the data presented in figure 6 give us the possibility to trace the mechanism of singlet-pair melting with increasing magnetic field. As follows from figure 6 at $h$ slightly above $h_{c1}$ spin singlet pairs start to melt in all antiferromagnetic bonds simultaneously and almost with the same intensity. With further increase of $h$, melting of weak AF bonds becomes more intense; however, at $h = h_{c_1}$, the process of melting stops. As seen in figure 6, weak AF bonds are polarized; however, their polarization is far from the saturation value $d_{s}^{w} \simeq 0.15$, while the strong AF bonds still manifest strong on-site singlet features with $d_{s}^{c} \simeq -0.65$. Postponement of the melting stops at $h = h_{c_1}$, but for $h > h_{c_1}$, strong AF bonds start to melt more intensively while the polarization of weak AF bonds increases slowly. Finally at $h = h_{c_2}$ both subsystems of AF bonds achieve an identical, almost fully polarized state. Note, that the almost symmetric fluctuations in on-AF-bond correlations increase in $d_{s}^{w}$ at $h \lesssim h_{c_1}$, decrease in $d_{s}^{c}$ at $h \gtrsim h_{c_1}$, and reflect the enhanced role of quantum fluctuations in the vicinity of quantum critical points.

In our previous paper [13], we introduced a mean field order parameter which can distinguish a gapless LL phase from the other gapped phases. This order parameter is the F-dimer order parameter which is defined as

$$P_{F} = \text{Re} \langle S_{n}^{-} S_{n+1}^{+} \rangle,$$  

The F-dimer order parameter has a considerable value in the Luttinger liquid phase and behaves differently in the other gapped phases. The effects of a small value of space modulation on this parameter are shown in figure 7. We have plotted $P_{F}$ versus magnetic field $h$ for chain of lengths $N = 12, 16, 20, 24$ with the exchange parameters $J_{F} = 1.0, J_{AF} = 9/2$, and $\delta = 1/9$. As can be seen, in the Haldane phase, $h < h_{c_2}$, the quantum fluctuations suppress the F correlations and the F-dimer parameter is close to zero value. Right after the first critical field, the F-dimer parameter increases rapidly up to the second critical field. In the intermediate region, $h_{c_1} < h < h_{c_2}$, the F-dimer parameter shows a non-zero plateau which behaves in the same way as the other parameters. By increasing the field, the F-dimer decreases and goes to zero at the saturation critical field $h = h_{c_2}$. The intermediate region is a gapped phase and we expect the zero value for the defined LL parameter, $P_{F}$. However, the gap does not affect the behavior of $P_{F}$ and a plateau appears in the curve.

5. Pair-wise entanglement

In this section we focus on the entanglement of two spins in different phases of the system. The entanglement which has no classical counterpart is employed to study the quantum correlations of different states. Concurrence is a measure of the bipartite entanglement which is defined as [40, 41]

$$C_{lm} = 2 \max\{0, C_{lm}^{(1)}, C_{lm}^{(2)}\},$$  

Figure 6. The AF bond dimerization order parameter as a function of the applied field $h$ for chains with exchanges $J_{F} = 1.0, J_{AF} = 9/2$, and $\delta = 1/9$ and lengths $N = 20, 24, 28$.

Figure 7. The F-dimer order parameter as a function of the applied field $h$, for the chains with exchanges $J_{F} = 1.0, J_{AF} = 9/2$, and $\delta = 1/9$ and lengths $N = 12, 16, 20, 24$. The appearance of a non-zero plateau in the curve is clear.
where
\[
C^{(1)}_{lm} = \left\{ \begin{array}{l}
\left( g_{lm}^{xx} - g_{lm}^{yy} \right)^2 + \left( g_{lm}^{yy} + g_{lm}^{zz} \right)^2 \\
- \frac{1}{4} - g_{lm}^{zz} \left( \frac{M_l^z - M_m^z}{2} \right)^2
\end{array} \right.
\]
and
\[
g_{lm}^{ab} = \langle S_l^a S_m^b \rangle
\]

is the correlation function between spins \( l \) and \( m \). The numerical Lanczos results on the concurrence for the 1D tetrameric spin-1/2 model are shown in figure 8. We have plotted the entanglement of two spins which are located at the same strong, weak, and F bond versus \( h \), chain length \( N = 28 \), and the exchange parameters \( J_F = 1.0, J_{AF} = 9/2, \) and \( \delta = 1/9 \). In the Haldane phase, \( h < h_c \), the spins on all AF bonds make a singlet state. In this state which is a maximally entangled state, \( g_{lm}^{xx} = g_{lm}^{yy} = g_{lm}^{zz} = \frac{1}{2} \). \( C^S = C^W = 1 \) and \( C^F \) is zero. For \( h > h_c \), the values of \( C^S \) and \( C^W \) fall down with increasing magnetic field. Indeed the quantum correlations of the two spins with strong AF and weak F interactions are decreased by increasing the magnetic field. However, an enhancement on the entanglement of the two spins with ferromagnetic interaction (SF) is observed. It means that the magnetic field increases the quantum correlations of the two spins which are interacting ferromagnetically. This is a dual effect of the magnetic field which increases the quantum correlations of two SFs and decreases the quantum correlations of two weak antiferromagnets (SWAs) and two strong antiferromagnets (SSAs). In the intermediate gapless region \( h_c < h < h_c^* \), the quantum correlations of SWAs and SSAs diminish down to \( h = h_c^* \) and the concurrences \( C^W \) and \( C^S \) reduce to \( \sim 0.1 \) and \( \sim 0.9 \) respectively. However, the quantum correlations of SF grow up to the critical field \( h_c \) and the entanglement reaches the value \( \sim 0.25 \). At the plateau state, the gap of the system is reopened and a plateau emerges in the curve of concurrences. In the intermediate gapped phase the values of the concurrences \( C^S, C^W, \) and \( C^F \) are 0.9, 0.1, and 0.25, respectively. Indeed in the plateau state there are three types of quantum correlations in the system. These correlators are the source of the mid-plateaus in the different parameters of the system such as magnetization, bond-dimer, and F-dimer parameters. Indeed all of these quantum correlators exist only at the mid-plateau states. In the full saturated state all of them disappear and the entanglement of the state is exactly zero.

To see the finite size effects, we have plotted in the inset of figure 8(a) the concurrence between two SSAs as a function of \( h \) for different chain sizes \( N = 16, 20, 24 \), and 28. It can be seen that there is no size effect on the numerical results and the concurrence behaves as a thermodynamic limit in the gapped regions.

To get more insight into the mid-plateau state, we have computed numerically the entanglement between the spins with different separation distances. The concurrence between an SSA and an arbitrary spin, say \( S_m \), has been plotted versus the separation distance \( m \), in figure 8(b). The entanglement of two such spins is decreased by increasing \( m \) and goes to zero at the finite value of \( m = 7 \). The same behavior is observed for the entanglement between an SWA and the spin \( S_m \) with respect to \( m \). The entanglement between SWAs and \( S_m \) goes to zero at \( m = 9 \). This means that in the plateau state the range of the quantum correlations between an SWA and \( S_m \) is longer than the range between an SSA and \( S_m \). This is the other feature of the mid-plateau state.

It is also remarkable that from our numerical results we found that the concurrence of two spins that are not on the same bond is equal to zero in the gapped Haldane and saturated F phases, which is in complete agreement with the analytical results.

6. Conclusion
In this paper, we have focused on the magnetic properties of a bond alternating antiferromagnetic–ferromagnetic spin-1/2
Heisenberg chain. Using two analytical approaches and a numerical method we have studied the effects of an external magnetic field and a space modulation on the ground state properties of the system. In the limit where the antiferromagnetic couplings are dominant, we mapped the model (1) to an effective XXZ Heisenberg chain with anisotropy parameter $\Delta = 1/2$ in the presence of effective uniform and staggered longitudinal magnetic fields. This model has different quantum phases which are distinguished by four critical fields. To find the critical fields we employed two field theoretical approaches: the nonlinear $\sigma$ model and bosonization, and the numerical exact diagonalization Lanczos method. Working on the spin coherent states representation, we mapped the model (1) to a nonlinear $\sigma$ model with an additional topological term. The topological term is dependent on the space modulation $\delta$ and the parameter $\alpha = \frac{J}{J_{AF}}$. For any values of $\alpha$ and $\delta$, the Hamiltonian mapped to a non-integrable $O(3)$ nonlinear $\sigma$ model with $\theta$ in the interval $[0, \pi]$. In the absence of a magnetic field the model is always gapped and the gap value depends on $\alpha$ and $\delta$. By analyzing our nonlinear $\sigma$ model in the presence of the magnetic field, we obtained only the two critical fields. To dominate this vacancy and to find the other two critical fields we also bosonized the effective Hamiltonian of the XXZ chain (3). Our bosonization procedure showed that the width of the mid-plateau is a function of $\delta J_{AF}$. It has been shown that the plateau width scales as a power low with exponent value 2 and vanishes at $\delta = 0$.

Moreover, we implemented the Lanczos method to numerically diagonalize chains with finite length up to $N = 28$. Using the exact diagonalization technique, we calculated the energy gap, magnetization, the string, the F-dimer, and the bond-dimer order parameters and various correlation functions for different values of the external magnetic field. In good qualitative agreement with our analytical results, we showed clearly that a space modulation on the antiferromagnetic exchanges leads to generation of a gap in the excitation spectrum of the system and, correspondingly, a magnetization mid-plateau at $\frac{N}{N_{ex}} = \frac{1}{4}$. We found that a non-zero plateau also creates in the plot of the F-dimer, bond-dimer order parameters.

To obtain more physical insight into the mid-plateau state we also investigated the pair-wise entanglement between two different spins of the system. As a measure of entanglement, the concurrence between two arbitrary spins was computed as a function of magnetic field. A plateau also appeared in the concurrence at the middle gapped state. In the plateau state there are three types of quantum correlations in the system. In the plateau state the range of the quantum correlations between a spin on the weak antiferromagnetic bond and a $S_0$ is longer than the range of the quantum correlations of a spin on the strong antiferromagnetic bond and $S_0$.

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