

Valence bond mapping of antiferromagnetic spin chains

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Boson mapping techniques are developed to describe valence bond correlations in quantum spin chains. Applying the method to the alternating bond Hamiltonian for a generic spin chain, we derive an analytic expression for the transition points which gives perfect agreement with existing density-matrix renormalization-group and quantum Monte Carlo calculations. [S0163-1829(97)03542-X]

Antiferromagnetic spin chains have been the subject of intense interest in recent years, largely due to the conjecture by Haldane¹ that chains built from integer spins should exhibit a gap in their energy spectrum. The existence of this gap, originally predicted on the basis of simple field-theoretic considerations, was subsequently confirmed experimentally.²

Much insight into the properties of antiferromagnetic spin chains has been provided by simple models. The field-theoretic nonlinear sigma model (NLSM),^{1,3} for example, provided the original motivation for Haldane's conjecture. Equally illuminating insight into the diverse properties of spin chain systems has been provided by the introduction of the valence bonds solid (VBS) state.⁴

Detailed descriptions of these systems, however, have depended on very complex numerical analyses, using either quantum Monte Carlo (QMC) simulations⁵ or density-matrix renormalization-group (DMRG) methods.⁶ These "exact" treatments provide striking confirmation of the features conjectured by Haldane.

Ideally, it would be nice to have a simpler method for a reliable quantitative treatment of quantum spin chains. Valence bonds provide a physically motivated starting point for such a description. The VBS is the exact ground state of specific spin-chain Hamiltonians involving quadratic and quartic terms, suggesting that wave functions constructed in terms of valence bonds might be good trial states more generally. Unfortunately, such wave functions are still too complex, for reasons to be discussed later, to be of general use in a variational analysis. In the present work, we propose a method that permits valence bonds to be used efficiently in variational calculations. The method makes use of boson mapping techniques, whereby a mapping is carried out to a space in which a valence bond is represented exactly by a boson.

We also report here an application of this method to study the phase transitions in spin chains governed by the alternating bond Hamiltonian.⁷ In this application, we consider an especially simple variational ansatz for the different phases of the system. Nevertheless, we find that our analysis reproduces perfectly the "exact" results for the critical points obtained in DMRG and QMC calculations.

A trial wave function containing the same physics was also considered recently in another variational analysis⁸ of the alternating bond Hamiltonian. There, however, the analysis was carried out without resorting to a valence bond boson mapping. We will discuss a bit further the relation between these two variational treatments later, after presenting the detailed results.

A useful starting point for the introduction of valence bonds is through the Schwinger boson realization of the spin algebra.⁹ The basic idea is to introduce a set of boson creation and annihilation operators $\gamma_{i,\sigma}^\dagger$ and $\gamma_{i,\sigma}$, respectively. These operators create and annihilate, respectively, a spin- $\frac{1}{2}$ boson with spin projection $\sigma = +\frac{1}{2}$ (denoted $+$) or $\sigma = -\frac{1}{2}$ (denoted $-$) at site i . A spin- S system would then involve $2S$ Schwinger bosons on each site.

Typical spin-chain Hamiltonians involve spin-spin interactions between nearest neighbors. It is natural therefore to consider states built up in terms of bonds reflecting these correlations. This is the basic idea behind the introduction of valence bonds. When dealing with an antiferromagnetic spin chain, the key correlations involve nearest neighbors in singlet states, which can be represented by the singlet bond

$$\Gamma_i^\dagger = \frac{1}{\sqrt{2}} (\gamma_{i,+}^\dagger \gamma_{i+1,-}^\dagger - \gamma_{i,-}^\dagger \gamma_{i+1,+}^\dagger). \quad (1)$$

In terms of these singlet bonds, the VBS ground state for a spin- S chain (S an integer) is given by

$$|\text{VBS}\rangle = \prod_{i=1,N} (\Gamma_i^\dagger)^S |0\rangle. \quad (2)$$

The state $|\text{VBS}\rangle$ is the exact ground eigenstate of the Hamiltonian

$$H = \sum_i \left[S_i \cdot S_{i+1} + \frac{1}{3} (S_i \cdot S_{i+1})^2 \right] \quad (3)$$

involving quadratic and quartic spin operators. For a general Hamiltonian, however, it is not an eigenstate. Furthermore, when not an exact eigenstate, it is not an especially useful trial state. The reason is that the singlet bonds Γ_i^\dagger from which

it is built are not bosons, i.e., the corresponding operators do not satisfy boson commutation relations.

This is a familiar problem in many branches of physics. A standard approach to problems of this type, involving dominant pair correlations, is to implement a *boson mapping*.¹⁰

The general idea of a boson mapping is to replace the original problem involving pair degrees of freedom (in this case, singlet bonds) and the true Hamiltonian of the system by an *equivalent* problem involving real bosons and an appropriate effective Hamiltonian for these bosons. All of the exchange effects between the constituents is transferred to the effective Hamiltonian, in a mathematically rigorous way guaranteed to preserve the physics of the original problem.

In more detail, we wish to *replace* the valence bonds $\gamma_{i,\sigma_1}^\dagger \gamma_{i+1,\sigma_2}^\dagger$ by bosons $B_{i,\sigma_1\sigma_2}^\dagger$, which fulfill exact bosonlike commutation relations:

$$[B_{i,\sigma_1\sigma_2}, B_{j,\sigma_3\sigma_4}^\dagger] = \delta_{i,j} \delta_{\sigma_1,\sigma_3} \delta_{\sigma_2,\sigma_4}. \quad (4)$$

There are many ways to implement such a replacement. In the generalized Holstein-Primakoff (GHP) approach,¹⁰ which we follow here, the mapping is defined by imposing the requirement that all quadratic operators in the original space are mapped in such a way as to preserve their commutation relations. More specifically, the boson image of quadratic operators are assumed to be given by *Taylor-series expansions*:

$$F_B = F^{(0)} + F^{(1)} + F^{(2)} + \dots \quad (5)$$

The terms in these Taylor expansions are obtained via the condition that any commutation rule $[A, B] = C$ between the original set of quadratic operators must be preserved at each order of the expansion:

$$\begin{aligned} [A^{(0)}, B^{(0)}] &= C^{(0)}, \\ [A^{(0)}, B^{(1)}] + [A^{(1)}, B^{(0)}] &= C^{(1)}, \\ &\dots \end{aligned} \quad (6)$$

We should note here that boson mappings have typically been applied to systems of interacting fermions. However, there is no fundamental difficulty in applying them to systems of interacting bosons,¹¹ as in the problems under discussion.

We have succeeded in building an appropriate boson mapping of the Holstein-Primakoff type for valence bonds. In the present discussion, we simply present the relevant mapping equations, leaving more detailed discussion of the formalism to a subsequent publication.

The full algebra of quadratic operators in the Schwinger boson space includes both particle-hole (p-h) operators of the form $\gamma_{i\sigma}^\dagger \gamma_{j\sigma'}$ and particle-particle operators of the form $\gamma_{i\sigma}^\dagger \gamma_{j\sigma'}^\dagger$ and $\gamma_{i\sigma} \gamma_{j\sigma'}$.

For the purpose of treating the dynamics of spin-chain Hamiltonians, we only need to know how to map the on-site p-h operator $\gamma_{i,\sigma}^\dagger \gamma_{i,\sigma'}$ and the p-p operators involving bonds between neighboring sites, $\gamma_{i,\sigma}^\dagger \gamma_{i+1,\sigma'}^\dagger$ and $\gamma_{i,\sigma} \gamma_{i+1,\sigma'}$. The relevant images through first-order in the Taylor series expansion are as follows.

The boson image of the on-site particle-hole operator is

$$(\gamma_{i,\sigma_1}^\dagger \gamma_{i,\sigma_2})_B = \sum_{\sigma_3} \{B_{i,\sigma_1\sigma_3}^\dagger B_{i,\sigma_2\sigma_3} + B_{i-1,\sigma_3\sigma_1}^\dagger B_{i-1,\sigma_3\sigma_2}\}. \quad (7)$$

Note that the on-site p-h operator maps exactly onto a p-h operator in the ideal boson space, with no need for a series expansion.

The p-p operators involving nearest neighbor bonds do require infinite series expansions. The lowest (zeroth) order images are straightforwardly given by

$$(\gamma_{i,\sigma_1}^\dagger \gamma_{i+1,\sigma_2}^\dagger)_B^{(0)} = B_{i,\sigma_1\sigma_2}^\dagger \quad (8)$$

and

$$(\gamma_{i,\sigma_1} \gamma_{i+1,\sigma_2})_B^{(0)} = B_{i,\sigma_1\sigma_2}. \quad (9)$$

The first-order images are more complex, as they provide the first reflection of exchange effects of the (Schwinger boson) constituents between neighbor bonds. The required first-order image that fulfills the second line of Eq. (6) is given by

$$\begin{aligned} (\gamma_{i,\sigma_1}^\dagger \gamma_{i+1,\sigma_2}^\dagger)_B^{(1)} &= \frac{1}{2} \sum_{\sigma_3, \sigma_4} \{B_{i,\sigma_1\sigma_3}^\dagger B_{i,\sigma_4\sigma_1}^\dagger B_{i,\sigma_4\sigma_3} \\ &\quad + B_{i,\sigma_1\sigma_3}^\dagger B_{i+1,\sigma_2\sigma_4}^\dagger B_{i+1,\sigma_3\sigma_4} \\ &\quad + B_{i,\sigma_3\sigma_2}^\dagger B_{i-1,\sigma_4\sigma_1}^\dagger B_{i-1,\sigma_4\sigma_3}\}. \end{aligned} \quad (10)$$

The corresponding image associated with annihilation of a bond between nearest neighbors is obtained from Eq. (10) by Hermitian conjugation.

In fact, closing the algebra to first order requires inclusion of the p-h operator between next-to-nearest neighbor (i with $i+2$) sites. We will not discuss this any further here, as it does not impact on the analysis or results to follow.

There is one further complication that should be noted before considering the application of these methods. The mapping equations given above can be applied in several different ways to a given spin-chain Hamiltonian. One possibility is to express the two-body interaction entering the Hamiltonian in p-p form ($\gamma^\dagger \gamma^\dagger \gamma \gamma$) and to map using Eqs. (8)–(10). Alternatively, the Hamiltonian could first be transformed into p-h form ($\gamma^\dagger \gamma \gamma^\dagger \gamma$) and then mapped with Eq. (7). A third possibility, of course, is to map part of the Hamiltonian in p-h form and part in p-p form. Were we to do the resulting analysis *exactly* in the ideal boson space, all such approaches would be equivalent. In variational treatments, on the other hand, it is essential to map the Hamiltonian in such a way as to maintain the key correlation effects.

As a first (test) application of these methods, we consider a spin-chain system governed by the alternating bond Hamiltonian⁸

$$H(\alpha) = \sum_{i=1}^N [1 - (-)^i \alpha] S_i \cdot S_{i+1}. \quad (11)$$

This system has been studied extensively in the literature. For a given value of the spin, it exhibits a sequence of phase

TABLE I. Location of the crossing points for the alternating bond spin chain. In addition to the results of the present analysis, we present results from the nonlinear sigma model (NLSM), from ‘‘exact’’ numerical solution, and from the VBS variational analysis of Ref. 8. In the case of the exact analyses, only the nonnegative crossing points are shown. The ‘‘exact’’ results for $S=1$ are from Ref. 12, those for $S=3/2$ are from Ref. 13, and those for $S=2$ are from Ref. 14.

S	Exact	Present results	NLSM	Ref. 8
1	0.25 ± 0.01	$\pm 1/4$	$\pm 1/2$	$\pm 1/3$
3/2	$0, 0.42 \pm 0.02$	$0, \pm 2/5$	$0, \pm 2/3$	$0, \pm 7/13$
2	$0.05 < \alpha < 0.3, 0.5 < \alpha < 0.6$	$\pm 1/6, \pm 1/2$	$\pm 1/4, \pm 3/4$	$\pm 1/4, \pm 2/3$
5/2		$0, \pm 2/7, \pm 4/7$	$0, \pm 2/5, \pm 4/5$	
3		$\pm 1/8, \pm 3/8, \pm 5/8$	$\pm 1/6, \pm 1/2, \pm 5/6$	

transitions, associated with successive partial dimerization of the system. The locations of the crossing points corresponding to the dimer phase transitions have been accurately determined for low-spin systems using both quantum Monte Carlo and density-matrix renormalization-group methods. This, coupled with the fact that the precise locations of the crossing points have not been reproduced by any mean field or variational treatment to date, makes it an ideal testing ground for our approach.

The variational treatment we will apply to this system is based on singlet bonds only. Thus, following our earlier remarks, we must map the Hamiltonian so as to most efficiently reflect these bonds. The appropriate separation is

$$H(\alpha) = H_1(\alpha) + H_2(\alpha), \quad (12)$$

where

$$\begin{aligned} H_1(\alpha) &= \sum_{i=1}^N [1 - (-)^i \alpha] S_i^z S_{i+1}^z \\ &= \frac{1}{4} \sum_{i=1}^N [1 - (-)^i \alpha] \sum_{\sigma} \sigma \gamma_{i,\sigma}^{\dagger} \gamma_{i,\sigma} \\ &\quad \times \sum_{\sigma'} \sigma' \gamma_{i+1,\sigma'}^{\dagger} \gamma_{i+1,\sigma'}, \end{aligned} \quad (13)$$

and

$$\begin{aligned} H_2(\alpha) &= \frac{1}{2} \sum_{i=1}^N [1 - (-)^i \alpha] (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) \\ &= \frac{1}{2} \sum_{i=1}^N [1 - (-)^i \alpha] \sum_{\sigma} \gamma_{i,\sigma}^{\dagger} \gamma_{i+1,-\sigma}^{\dagger} \gamma_{i,-\sigma} \gamma_{i+1,\sigma}. \end{aligned} \quad (14)$$

We map the term $H_1(\alpha)$, corresponding to $S_i^z S_{i+1}^z$, in p-h form and the term $H_2(\alpha)$, corresponding to $S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+$, in p-p form.

Applying the mapping in this way to the alternating bond Hamiltonian (11) and then projecting onto singlet bosons, defined by

$$\sigma_i^{\dagger} = \frac{1}{\sqrt{2}} [B_{i,+}^{\dagger} - B_{i,-}^{\dagger}], \quad (15)$$

we obtain

$$\begin{aligned} H_B(\alpha) &= -\frac{1}{4} \sum_{i=1}^N [1 - (-)^i \alpha] \{ 3 \sigma_i^{\dagger} \sigma_i + \sigma_i^{\dagger} [\sigma_i^{\dagger} \sigma_i + \sigma_{i+1}^{\dagger} \sigma_{i+1} \\ &\quad + \sigma_{i-1}^{\dagger} \sigma_{i-1}] \sigma_i \}. \end{aligned} \quad (16)$$

The trial wave function we use in our variational description of the alternating bond spin-chain system is

$$|\Phi_{n_o, n_e}\rangle = \prod_{i(\text{odd})=1}^N \frac{\sigma_i^{\dagger n_o} \sigma_{i+1}^{\dagger n_e}}{\sqrt{n_o! n_e!}} |0\rangle, \quad (17)$$

subject to the Schwinger constraint

$$n_o + n_e = 2S. \quad (18)$$

This trial wave function reflects the various phases of the system. The Heisenberg phase corresponds to $n_o = n_e$, with all sites involved in an equal number of bonds with its nearest neighbors on each side. The corresponding state is translationally invariant and is the analogue of the VBS state in the ideal boson space. Increasing n_o or equivalently n_e corresponds to successive partial dimerization. The cases in which either $n_o = 0$ or $n_e = 0$ involve complete dimerization.

Here we focus our analysis on the location of the critical points associated with a transition from one phase to another. Defining

$$\mathcal{E}_{n_o, n_e}(\alpha) = \langle \Phi_{n_o, n_e} | H_B(\alpha) | \Phi_{n_o, n_e} \rangle, \quad (19)$$

the critical points are given by the condition

$$\mathcal{E}_{n_o, n_e} = \mathcal{E}_{n_o \pm 1, n_e \mp 1}. \quad (20)$$

Straightforward analysis yields for the energy functional,

$$\begin{aligned} \mathcal{E}_{n_o, n_e}(\alpha) &= -\frac{N}{4} \left[(1 + \alpha) \left\{ \frac{3n_o}{2} + \frac{n_o(n_o - 1)}{2} + n_o n_e \right\} \right. \\ &\quad \left. + (1 - \alpha) \left\{ \frac{3n_e}{2} + \frac{n_e(n_e - 1)}{2} + n_o n_e \right\} \right], \end{aligned} \quad (21)$$

and for the critical values of α ,

$$\alpha = \frac{2n_o + 1 - 2S}{2(S + 1)}, \quad n_o = 0, 1, \dots, 2S - 1. \quad (22)$$

In Table I, we present the results of this analysis for several values of the spin S . We compare the results obtained

from our simple analytic formula (22) for the crossing points with those from “exact” calculations,^{12–14} from the NLSM (Refs. 1 and 3) and from the recent VBS variational treatment of Ref. 8. Our simple formula, obtained by using a first-order boson mapping treatment and a simple product trial state, yields perfect agreement with the “exact” results where available. This is to be contrasted with the NLSM results, which are in much worse agreement. And, indeed, our results are even better than the results of Ref. 8, despite the similarity of the two variational approaches. Note that we have also included in the table *predictions* for the location of the phase transition points at higher spins.

It is worth expanding a bit on the relation between our variational treatment of the alternating bond Hamiltonian and the treatment of Ref. 8. As noted earlier, the two approaches include much the same physical content in their trial wave functions. In our view, our approach has several advantages. In our method, the various phases of the system are described by states that are inherently orthogonal. In contrast, the trial states used in Ref. 8 are only asymptotically orthogonal. Furthermore, our method is by no means limited to the use of the very simple trial wave functions of Eq. (17). The existence of a relatively simple boson Hamiltonian as output from the mapping makes it possible to extend the dynamical treatment to more complex wave functions. Thus, we can readily improve on our description of the ground state and also readily build excitations of the system, all

within the same basic framework. It is by no means evident how this can be done without implementation of the valence bond boson mapping.

Indeed, there is clearly room for improvement in our analysis of the alternating bond spin chain. From Eq. (21), we see that at the level of approximation we considered here the energy per site of the pure $S=1$ Heisenberg chain ($\alpha=0$) is $-5/4$. The accepted value is $-1.401\dots$,⁶ while the VBS variational result⁸ lies between the two at $-4/3$. We expect that the necessary improvement to our result would be provided in part by the next-order contribution of the boson mapping and in part by fluctuation effects. What is important to reiterate, however, is that the method we have outlined provides a systematic way to incorporate such improvements.

There are several areas in which we expect these methods to be useful in the future. Our immediate plan is to generalize the Hamiltonian (11) to include crystal fields and a uniform magnetic field and to study the phase diagram, excitations, magnetization curves, etc.

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