Valence Bond Mapping of Antiferromagnetic Spin Chains

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Abstract

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 (DMRG) and Quantum Monte Carlo (QMC) calculations.

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Antiferromagnetic spin chains have been the subject of intense interest in recent years, largely due to the conjecture by Haldane [1] 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 non-linear 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) simulations [5] 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 useful in a variational analysis. In the present work, we propose a method that permits valence bonds to be used efficiently in variational calculations. We also describe the application of this method to study the phase transitions in spin chains governed by the alternating bond hamiltonian [7].

A useful starting point for the introduction of valence bonds is through the Schwinger boson realization of the spin algebra [8]. The basic idea is to introduce a set of boson creation and annihilation operators $\gamma^\dagger_{i,\sigma}$ 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 spin-singlet states, which can be represented by the singlet bond

\[ \Gamma_i^+ = \frac{1}{\sqrt{2}} (\gamma_{i,+,i+1,-} - \gamma_{i,-,i+1,+}) . \] (1)

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

\[ |VBS> = \prod_{i=1,N} (\Gamma_i^+)^S |0> . \] (2)

The state |VBS> is the exact ground eigenstate of the hamiltonian

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

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 \( \gamma_{i,\sigma_1}^+ \gamma_{i+1,\sigma_2}^+ \) by bosons \( B_{i,\sigma_1\sigma_2}^+ \), which fulfill exact bosonlike commutation relations:
\[
[B_{i,\sigma_{1}\sigma_{2}}, B_{j,\sigma_{3}\sigma_{4}}^{\dagger}] = \delta_{i,j} \delta_{\sigma_{1},\sigma_{3}} \delta_{\sigma_{2},\sigma_{4}}. \tag{4}
\]

There are many ways to implement such a replacement. In the Generalized Holstein-Primakoff (GHP) approach [9], 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 \textit{Taylor-series expansions}:

\[
F_B = F^{(0)} + F^{(1)} + F^{(2)} + \ldots. \tag{5}
\]

- 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:

\[
[A^{(0)}, B^{(0)}] = C^{(0)}
\]

\[
[A^{(0)}, B^{(1)}] + [A^{(1)}, B^{(0)}] = C^{(1)}
\]

\[
\ldots. \tag{6}
\]

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 [10], 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 $\gamma_i^{\dagger} \gamma_i$, and the p-p operators involving bonds between neighboring sites, $\gamma_i^{\dagger} \gamma_{i+1}^{\dagger}$ and $\gamma_i \gamma_{i+1}$. 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:

$$\left( \gamma_i^{\dagger} \gamma_i \right)_B = \sum_{\sigma_3} \left\{ B_{i,\sigma_1 \sigma_2} B_{i,\sigma_3 \sigma_4} + B_{i-1,\sigma_1 \sigma_2} B_{i-1,\sigma_3 \sigma_4} \right\} .$$

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

$$\left( \gamma_i^{\dagger} \gamma_i^{\dagger} \gamma_i^{\dagger} \right)_B = B_{i,\sigma_1 \sigma_2} \quad (8)$$

and

$$\left( \gamma_i^{\dagger} \gamma_i \gamma_i^{\dagger} \right)_B = B_{i,\sigma_1 \sigma_2} \quad (9)$$

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 (6) is given by

$$\left( \gamma_i^{\dagger} \gamma_i^{\dagger} \gamma_{i+1}^{\dagger} \right)_B = \frac{1}{2} \sum_{\sigma_3,\sigma_4} \left\{ B_{i,\sigma_1 \sigma_2} B_{i,\sigma_3 \sigma_4} B_{i+1,\sigma_3 \sigma_4} + B_{i,\sigma_1 \sigma_2} B_{i+1,\sigma_3 \sigma_4} B_{i+1,\sigma_3 \sigma_4} \right\} .$$

The corresponding image associated with annihilation of a bond between nearest neighbors is obtained from (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 \((\gamma^\dagger \gamma \gamma^\dagger)\) and to map using eqs. (8-10). Alternatively, the hamiltonian could first be transformed into p-h form \((\gamma^\dagger \gamma \gamma^\dagger)\) 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 specific application of these methods, we consider a spin-chain system governed by the alternating bond hamiltonian \([7]\),

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

(11)

This system has been studied extensively, especially with regards to its dimer phase transitions.

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:

\[
H(\alpha) = H_1(\alpha) + H_2(\alpha) ,
\]  

(12)

where

\[
H_1(\alpha) = \sum_{i=1}^{N} [1 - (-)^i \alpha] S_i^z S_{i+1}^z
\]

\[
= \frac{1}{4} \sum_{i=1}^{N} [1 - (-)^i \alpha] \sum_{\sigma} \gamma_{i,\sigma}^\dagger \gamma_{i,\sigma} \sum_{\sigma'} \gamma_{i+1,\sigma'}^\dagger \gamma_{i+1,\sigma'} .
\]  

(13)

and

\[
H_2(\alpha) = \frac{1}{2} \sum_{i=1}^{N} [1 - (-)^i \alpha] (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) 
\]

\[
= \frac{1}{2} \sum_{i=1}^{N} [1 - (-)^i \alpha] \sum_{\sigma} \gamma_{i,\sigma}^\dagger \gamma_{i+1,-\sigma}^\dagger \gamma_{i,-\sigma} \gamma_{i+1,\sigma} .
\]  

(14)
We map the term $H_1(\alpha)$, corresponding to $S_i^+ S_{i+1}^-$, 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
\begin{equation}
\sigma_i^\dagger = \frac{1}{\sqrt{2}} [B_{i,+}^\dagger - B_{i,-}^\dagger] ,
\end{equation}
we obtain
\begin{equation}
H_B(\alpha) = -\frac{1}{4} \sum_{i=1}^{N} [1 - (-)^i \alpha] \left\{ 3\sigma_i^\dagger \sigma_i + \sigma_i^\dagger [\sigma_{i+1}^\dagger \sigma_{i+1} + \sigma_{i-1}^\dagger \sigma_{i-1}] \sigma_i \right\} .
\end{equation}

The trial wave function we use in our variational description of the alternating bond spin-chain system is
\begin{equation}
|\Phi_{n_o,n_e}\rangle = \prod_{i\text{(odd)}}^{N} \frac{\sigma_i^\dagger^{n_o} \sigma_{i+1}^\dagger^{n_e}}{\sqrt{n_o! n_e!}} |0\rangle ,
\end{equation}
subject to the Schwinger constraint
\begin{equation}
n_o + n_e = 2S .
\end{equation}

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
\begin{equation}
\mathcal{E}_{n_o,n_e}(\alpha) = \langle \Phi_{n_o,n_e} | H_B(\alpha) | \Phi_{n_o,n_e} \rangle ,
\end{equation}
the critical points are given by the condition
\begin{equation}
\mathcal{E}_{n_o,n_e} = \mathcal{E}_{n_o\pm1,n_e\mp1} .
\end{equation}
Straightforward analysis yields for the energy functional,

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

and for the critical values of \( \alpha \),

\[ \alpha = \frac{2n_o + 1 - 2S}{2(S + 1)}, \quad n_o = 0, 1, \ldots, 2S - 1. \quad (22) \]

In Table 1, 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 [11–13] and from the NLSM [1,3]. 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. Note that we have also included in the table predictions for the location of the phase transition points at higher spins.

The fact that our first-order boson mapping works so well in describing the location of dimer phase transitions does not mean that higher-order contributions are of no dynamical importance. Indeed, at the same level of approximation, the energy per site of the pure \( S = 1 \) Heisenberg lattice (\( \alpha = 0 \)) is calculated to be \(-5/4\), whereas the exact result is \(-1.401\ldots\) [6]. Thus, there is clearly room for improvement, which we expect would be provided in part by the next-order contribution of the boson mapping and in part by fluctuation effects. What is important to realize, 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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REFERENCES

[1] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).

[2] W. J. L. Buyers, R. M. Morra, R. L. Armstrong, P. Gerlach and K. Hirakawa, Phys. Rev. Lett. **56**, 371 (1986); J. P. Renard, M. Verdaguer, L. P. Regnault, W. A. C. Erkelens, J. Rossat-Mignod and W. G. Stirling, Europhys. Lett. **3**, 945 (1987).

[3] I. Affleck, Nucl. Phys. **B257**, 397 (1985).

[4] I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).

[5] S. Liang, Phys. Rev. Lett. **64**, 1597 (1990).

[6] Steven R. White and David A. Huse, Phys. Rev. **B48**, 3844 (1993).

[7] I. Affleck and F. D. M. Haldane, Phys. Rev. **B36**, 5291 (1987).

[8] Daniel P. Arovas, Assa Auerbach and F. D. M. Haldane, Phys. Rev. Lett. **60**, 531 (1988).

[9] Abraham Klein and E. R. Marshalek, Rev. Mod. Phys. **63**, 375 (1991).

[10] R. Bijker, S. Pittel and J. Dukelsky, Phys. Lett. **219B**, 5 (1989); J. Dukelsky and S. Pittel, Phys. Rev. **C39**, 2001 (1989).

[11] Y. Kato and A. Tanaka, J. of Phys. Soc. Jap. **63**, 1277 (1994).

[12] M. Yajima and M. Takahashi, J. of Phys. Soc. Jap. **65**, 39 (1996).

[13] Masanori Yamanaka, Masaki Oshikawa and Seiji Miyashita, J. of Phys. Soc. Jap. **65**, 1562 (1996).
TABLES

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 non-linear sigma model (NLSM) and from “exact” numerical solution. In the case of the exact analyses, only the nonnegative crossing points are shown.

| S   | Exact               | Present Results | NLSM    |
|-----|---------------------|-----------------|---------|
| 1   | 0.25 ±0.01          | ±1/4            | ±1/2    |
| 3/2 | 0. , 0.42 ±0.02     | 0 , ±2/5        | 0 , ±2/3|
| 2   | 0.05< α <0.3 , 0.5< α <0.6 | ±1/6 , ±1/2 | ±1/4 , ±3/4 |
| 5/2 | —                   | 0 , ±1/3 , ±2/3 | 0 , ±2/5 , ±4/5 |
| 3   | —                   | ±1/7 , ±3/7 , ±5/7 | ±1/6 , ±1/2 , ±5/6 |

The exact results for $S = 1$ are from Ref. 11, those for $S = 3/2$ are from Ref. 12, and those for $S = 2$ are from Ref. 13.