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A UNIFIED MANY-BODY THEORY OF HAMILTONIAN LATTICE SYSTEMS

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Abstract. In this article we review our recent applications of a powerful, nonperturbative, quantum-mechanical many-body technique, namely the coupled-cluster method (CCM), to several quantal spin-lattice systems exhibiting antiferromagnetism in some phases, and to various lattice gauge field models in several dimensions. In particular, a unified formalism is developed for these lattice problems within the CCM framework, in order to investigate the ground-state properties and the low-lying excitations.

1. INTRODUCTION

The coupled-cluster method (CCM) was invented some 35 years ago to study the strong correlations between nucleons in closed-shell atomic nuclei [1]. Since then its applications have been extended to a wide range of problems in physics and chemistry. These include many-body problems in atoms and molecules, finite nuclei (including open-shell nuclei) and nuclear matter, the electron gas, various quantum field theories and impurity problems. The interested reader is referred to Ref. [2] and the references cited therein for an overview of the method and its applications to date. Since the CCM has become increasingly recognized over the last decade as providing one of the most powerful, most versatile, and potentially most accurate of all formulations of the quantum many-body problem, it is perhaps not surprising that during the last few years the method has been extended to deal with such quantum lattice problems of topical interest as spin-lattice systems [3] and lattice gauge field theory [4]. In view of the success of these preliminary applications, it is our intention in the present article

to show how the CCM can be regarded as providing a unified theory for the treatment of quantum-mechanical Hamiltonian lattice systems.

Even quantum-mechanical spin-lattice systems with very simple Hamiltonians are often endowed with very complex physical properties and rich phase diagrams. Furthermore, their behaviour is often counter-intuitive and quite unlike that of their classical counterparts. Particularly well-known examples are the one-dimensional (1D) spin- $\frac{1}{2}$ Heisenberg model, which is fully integrable by the Bethe *ansatz* [5] (and from which it is known to have a gapless excitation spectrum), and its non-integrable spin-1 counterpart, which has been conjectured by Haldane [6] to have a nonzero gap. By varying the combinations of interactions (e.g., nearest-neighbour and next-nearest-neighbour interactions, with or without anisotropy), the lattice structure, the spin of the particles, the dimensionality of the system, and such other externally applied parameters as the magnetic field, such quantal spin systems can exhibit a bewildering array of orderings and phase structures. These include, for example, phases with Ising-like long-range order, dimerized or trimerized phases, quantum spin fluids and many other exotic and often still ill-understood structures.

In view of the above, and because a number of exact solutions are also known for a variety of models for at least certain values of their coupling constants, these spin-lattice systems therefore provide a particular challenge for the quantum many-body theorist to provide an accurate and detailed *ab initio* microscopic description of their properties. Furthermore, the importance of this challenge has been focused by the realization that the 2D spin- $\frac{1}{2}$ lattice systems have special relevance to the ceramic cuprate and allied materials exhibiting high-temperature superconductivity.

Lattice gauge field theory was developed to provide a cure for the chronic divergence problems of quantum field theories in continuous space. Nowadays, lattice gauge models are interesting not only in their own right but also because they provide a particularly stringent test for theoretical techniques due to their inherently nonperturbative character and the strict need to incorporate gauge-invariance at all stages. Nevertheless, lattice gauge field theory shares many of the features of spin-lattice models. In this paper we exploit this similarity, and show how various lattice approximation schemes developed for the spin models can be modified rather easily for use with both Abelian and non-Abelian lattice gauge models. We show in particular how we are thereby able to obtain good results for the ground-state energy for various values of the coupling parameters ranging from strong to weak.

In this article, we review our CCM results for such spin-lattice systems as the anisotropic Heisenberg (or XXZ) model and such lattice gauge theories as the $U(1)$ model of quantum electrodynamics, both of which are described in Sec. 2. We focus especially on the ground states here, and aim to demonstrate that the CCM provides an effective and unified technique to deal with such lattice problems as the above archetypal examples. We also outline some future prospects of our CCM analysis for both several exotic phases of other spin models and such non-Abelian lattice gauge theories as the $SU(2)$ model.

The remainder of the paper is organized as follows. Correlations in the CCM, as in any other microscopic description, are described with respect to some suitable (uncorrelated or) model state, as explained in Sec. 2. Our initial application of the CCM to spin-lattice problems started with an interest in the antiferromagnetic Ising-like phase where the classical Néel state would appear to be a good *a priori* choice of

model state. In Sec. 3 we consider the XXZ model Hamiltonian, and apply to it two different systematic hierarchical approximation schemes in a CCM description based on the Néel state as model state. One scheme includes correlations of arbitrarily long range in each order of implementation, thereby permitting possible phase transition to be predicted. The other scheme is a local approximation scheme in which many-body correlations involving considerably more spins than in the former scheme can be calculated with very high accuracy. We also demonstrate in Sec. 3 how the CCM can be adapted to incorporate a different choice of model state (namely, here, the planar model state), by reference to the particular example of the 1D spin-1 Heisenberg-biquadratic model. Analogues of the above CCM truncation schemes for the $U(1)$ lattice gauge theory are demonstrated in Sec. 4, where we also discuss alternative choices of model state. In Sec. 5 we consider very briefly the possible extension of this work to the non-Abelian $SU(2)$ model, and in Sec. 6 we conclude with a critical discussion of the results attained to date, and the potential of the CCM for wider application.

2. COUPLED-CLUSTER FORMALISM FOR LATTICE PROBLEMS

2.1 Basic Ingredients

As stated in Sec. 1, the coupled-cluster method (CCM) was developed for the study of many-body correlations in a quantum system. To achieve this the CCM first focuses on the exact many-body wavefunction $|\Psi_g\rangle$ for the ground ket state. The starting point for a coupled-cluster description is the model (or reference) state $|\Phi\rangle$. Although there is considerable freedom in its choice, the usual primary requirement on it has been that it is a cyclic vector, with respect to which one may define two mutually commuting subalgebras of multiconfigurational creation operators $\{C_I^\dagger\}$ and their Hermitian-conjugate destruction counterparts $\{C_I\}$. The set-index I labels a general multiparticle cluster configuration with respect to the state $|\Phi\rangle$ in the role of vacuum or reference state. The operators $\{C_I^\dagger\}$ and $\{C_I\}$ are complete in the sense that arbitrary ket and bra states within the many-body Hilbert space may be decomposed as the respective linear combinations

$$|\Psi\rangle = \sum_I \psi_I C_I^\dagger |\Phi\rangle; \quad \langle\tilde{\Psi}| = \sum_I \tilde{\psi}_I \langle\Phi| C_I. \quad (2.1)$$

In the CCM the multiparticle correlations in the ground ket state are in principle included exactly in terms of an *exponentiated* cluster correlation operator S ,

$$|\Psi_g\rangle = e^S |\Phi\rangle; \quad H|\Psi_g\rangle = E_g |\Psi_g\rangle, \quad (2.2)$$

which may be decomposed wholly in terms of creation operators

$$S = \sum_I' S_I C_I^\dagger, \quad (2.3)$$

where, by definition, the prime on the sum over configurations $\{I\}$ excludes the $I = 0$ term corresponding to the identity operator, $C_0^\dagger \equiv 1$. We thus have the

intermediate normalization condition $\langle \Phi | \Psi_g \rangle = \langle \Phi | \Phi \rangle = 1$, in the usual scheme where $\langle \Phi | C_I^\dagger | \Phi \rangle = 0$, $\forall I \neq 0$. The correlation operator of an N -body system may itself also be decomposed as a linear superposition of n -body partitions, $S = \sum_{n=1}^N S_n$, where S_n describes the configurations formed by exciting n particles from their single-particle states contained in $|\Phi\rangle$.

The reason for writing the correlations in the exponential form of Eqs. (2.2) and (2.3), rather than in the linear form of Eq. (2.1) typical of the configuration-interaction method, lies at the very heart of the CCM, as described more fully in Ref. 2. We only recall here that the exponential form leads to: (i) a proper counting of *independent* excitations (e.g., n independent pairs of particles excited from $|\Phi\rangle$) are properly described by the wavefunction $\frac{1}{n!}(S_2)^n|\Phi\rangle$; (ii) the automatic incorporation of the important Goldstone linked-cluster theorem; and (iii) hence also a proper scaling with particle number N (i.e., size-extensivity) of such extensive variables as the ground-state energy E_g in the infinite limit, $N \rightarrow \infty$.

Practical implementations of the CCM are made by restricting the cluster amplitudes $\{S_I\}$ to some (finite or infinite) subset of the entire set, within a well-defined hierarchy of approximations. The retained amplitudes are then solved for approximately, as follows. The ground-state Schrödinger equation of Eq. (2.2) is first rewritten in the similarity-transformed form,

$$(e^{-S} H e^S - E_g) |\Phi\rangle = 0, \quad (2.4)$$

which is the hallmark of the CCM. By taking the inner products of Eq. (2.4) with the complete set of states consisting of $|\Phi\rangle$ itself and $\{C_I^\dagger |\Phi\rangle; I \neq 0\}$, we find respectively,

$$\langle \Phi | e^{-S} H e^S | \Phi \rangle = E_g, \quad (2.5)$$

and

$$\langle \Phi | C_I e^{-S} H e^S | \Phi \rangle = 0; \quad I \neq 0. \quad (2.6)$$

The set of equations (2.6) represents a coupled set of nonlinear equations for the c -number coefficients $\{S_I\}$, equal in number to the number of retained coefficients, and, in terms of the solution to which, Eq. (2.5) gives the ground-state energy, $E_g = E_g[S_I]$.

Due to the nested commutator expansion,

$$e^{-S} H e^S = H + [H, S] + \frac{1}{2!} [[H, S], S] + \dots, \quad (2.7)$$

and the fact that each of the individual components of S commutes with all others, every element of S in Eq. (2.3) is linked directly to the Hamiltonian in each of the terms in Eq. (2.7). Hence, each of the coupled equations (2.6) is of the linked-cluster type. Furthermore, the otherwise infinite series of Eq. (2.7) actually terminates after a finite number of terms if, as is usually the case, each term in the second-quantized form of the Hamiltonian contains a finite number of single-particle destruction operators defined with respect to $|\Phi\rangle$. Equations (2.5) and (2.6) are therefore of finite order in the retained coefficients $\{S_I\}$, and need no additional (artificial or approximate) truncation. In this very important respect the CCM differs from its unitary-transformation counterpart that would arise in a standard variational formulation, in

which the bra state $\langle \Psi_g |$ is simply taken as the manifest Hermitian conjugate of $|\Psi_g\rangle$. This feature is important, and leads naturally to the biorthogonal CCM description (rather than the more usual orthogonal one) in which the manifest Hermitian conjugacy of corresponding bra and ket states is lost. While the bra states are not needed to calculate the ground-state energy, they *are* needed to calculate such other ground-state expectation values as order parameters. Since we concentrate here only on the ground-state energies of spin-lattice and lattice gauge field models, we refer the reader to Ref. [2] and the references cited therein for further details of the bra-state CCM parametrization.

In the remainder of this section we illustrate the above general formalism for the specific cases of the XXZ spin-lattice model and $U(1)$ lattice gauge field theory.

2.2 The XXZ Spin-Lattice Model

The XXZ or anisotropic Heisenberg model is an archetypal spin-lattice problem. It comprises N spins (with spin quantum number s) on the sites $\{i\}$ of a d -dimensional regular lattice, which interact via nearest-neighbour couplings described by the Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^N \sum_{\rho=1}^z \left[\Delta s_i^z s_{i+\rho}^z + \frac{1}{2} (s_i^+ s_{i+\rho}^- + s_i^- s_{i+\rho}^+) \right], \quad (2.8)$$

where the index i runs over all N ($\rightarrow \infty$) lattice sites with the usual periodic boundary condition imposed; the index ρ runs over all z nearest-neighbour sites (i.e., z is the coordination number of the lattice); the operators s_i^z and $s_i^\pm \equiv s_i^x \pm i s_i^y$ are spin- s operators obeying the usual $SU(2)$ angular momentum commutation relations; and Δ is the anisotropy parameter, which in the special case $\Delta = 1$ gives the isotropic Heisenberg Hamiltonian. For present purposes we consider only the case of bipartite lattices, where the lattice is composed of two alternating sublattices, which we denote as A and B . Bipartite lattices include the important examples of the 1D chain, 2D square lattice, and, more generally, the hypercubic lattice in any number of dimensions. The restriction to bipartite lattices excludes such lattices as the triangular lattice and sidesteps the associated effects of frustration. Furthermore, we restrict our attention in this article to the case $\Delta > 0$, where the system is known to be antiferromagnetic, for example, for the spin- $\frac{1}{2}$ 1D chain.

Let us first consider the limiting case of the Ising model, where $\Delta \rightarrow \infty$. In this limit the ground state of Eq. (2.8) is clearly given by the (classical) Néel state $|N2\rangle$ in which all spins on the A -sublattice have z -component $s^z = -s$, say, and all of those on the B -sublattice have $s^z = +s$. The Néel state thus has perfect antiferromagnetic long-range order. In order to study the quantum correlations at any finite Δ , it seems appropriate to take the Néel state as our reference state $|\Phi\rangle$ in a CCM analysis. The correlation effects are thus incorporated by considering excitations with respect to the above model Néel state. The single-spin creation operators with respect to this state are clearly the spin-raising operators s_i^+ for sites i on the "spin-down" A -sublattice, and the spin-lowering operators s_j^- for sites j on the "spin-up" B -sublattice. Each operator can act a maximum of $2s$ times on a single site before the Néel state is annihilated.

We also note that the Hamiltonian of Eq. (2.8) commutes with the operator $s_{\text{total}}^z (\equiv \sum_{i=1}^N s_i^z)$, and that the antiferromagnetic ground state $|\Psi_g\rangle$ may therefore, by definition, be sought in the restricted subspace where $s_{\text{total}}^z = 0$. We may thus write

$$|\Psi_g\rangle = e^S |N2\rangle; \quad S = \sum_{n=1}^{N/2} S_{2n}, \quad (2.9)$$

with the correlation operators S_{2n} given, with a somewhat arbitrary choice of normalization constant, as

$$S_{2n} = \frac{(-1)^n}{(n!)^2} \sum_{i_1, i_2, \dots, i_n} \sum_{j_1, j_2, \dots, j_n} S_{i_1 i_2 \dots i_n j_1 j_2 \dots j_n} s_{i_1}^+ s_{i_2}^+ \dots s_{i_n}^+ s_{j_1}^- s_{j_2}^- \dots s_{j_n}^-, \quad (2.10)$$

where we have used indices $\{i_l\}$ and $\{j_m\}$ for sites on the A - and B -sublattices, respectively. Clearly, for spin- s particles, the coefficients $S_{i_1 i_2 \dots i_n j_1 j_2 \dots j_n}$ in Eq. (2.10) are non-vanishing only when a given lattice index appears no more than $2s$ times.

The ground-state energy per particle in this case is rather straightforwardly calculated from Eq. (2.5) as,

$$\frac{E_g}{N} = -\frac{zs^2}{2}(\Delta + 2b_1), \quad (2.11)$$

where z is the coordination number of the lattice and $b_1 \equiv S_{i, i+\rho}$ is the nearest-neighbour pair correlation coefficient. We note that b_1 is independent of both the index i by translational invariance, and the index ρ by the lattice symmetries under rotations and reflections. We also note that Eq. (2.11) is *exact*, and that b_1 is itself determined by the coupled set of equations (2.6), which become in the present case,

$$\langle \Phi | s_{i_1}^- s_{i_2}^- \dots s_{i_n}^- s_{j_1}^+ s_{j_2}^+ \dots s_{j_n}^+ e^{-S} H e^S | \Phi \rangle = 0, \quad n = 1, 2, \dots, N/2. \quad (2.12)$$

In any practical calculation one has to make either a finite or infinite truncation of the expansion for the correlation operator S given by Eqs. (2.9) and (2.10) in order to determine the otherwise infinite number of correlation coefficients $\{S_{i_1 \dots i_n j_1 \dots j_n}\}$. A number of such truncation schemes are now available, some of which are discussed further in Sec. 3. Finally, Eqs. (2.12) are to be evaluated, one for each retained correlation coefficients, and then solved. Such explicit evaluation can rapidly become tedious and time-consuming if done by hand. Nevertheless, the process is very amenable to automation using computer-algebraic techniques.

2.3 $U(1)$ Lattice Gauge Field Theory

The Hamiltonian lattice gauge field theory is usually defined in d spatial dimensions on a d -dimensional hypercubic lattice. Thus, the theory is defined in one dimension (1D) on an $N \times 1$ array of elementary (1×1 square) plaquettes, in two dimensions (2D) on an $N \times N$ square array of plaquettes, in three dimensions (3D) on an $N \times N \times N$ cubic array of plaquettes, etc. For example, the Hamiltonian for the $U(1)$ lattice gauge field theory is defined in the vacuum sector in terms of a coupling constant λ as

$$H = \frac{1}{2} \sum_i \frac{\partial^2}{\partial A_i^2} + \lambda \sum_p (1 - \cos B_p), \quad (2.13)$$

and the Hamiltonian for the non-Abelian $SU(2)$ model will be discussed in Sec. 5. In Eq. (2.13), the vector potential A_l is defined on the links l of the lattice, whereas the magnetic field B_p is a plaquette variable defined by the four values of A_l with $l \in p$ on the elementary plaquette as the lattice curl, namely

$$B_p \equiv A_1 + A_2 - A_3 - A_4, \quad (2.14)$$

where the order for the four link indices is counterclockwise around the plaquette p , and the overall sign is chosen by convention. In the compact $U(1)$ theory B_p is constrained to lie in the range $-\pi \leq B_p \leq \pi$.

For practical calculations, it is very useful to express Eq. (2.13) in terms of plaquette variables alone. For both the 1D array and the 2D square lattice, it is easy to show that

$$H = \sum_{p=1}^{N_p} \left[-2 \frac{\partial^2}{\partial B_p^2} + \lambda(1 - \cos B_p) \right] + \frac{1}{2} \sum_{p,\rho} \frac{\partial^2}{\partial B_p \partial B_{p+\rho}}; \quad -\pi \leq B_p \leq \pi, \quad (2.15)$$

where N_p is the number of plaquettes in the lattice and ρ is, as before, a lattice vector connecting nearest-neighbour plaquettes of the lattice.

In lattice gauge field theory, the case $\lambda \rightarrow 0$ is usually referred to as the strong-coupling limit, while the case $\lambda \rightarrow \infty$ is termed the weak-coupling limit. In the strong-coupling limit ($\lambda = 0$), the Hamiltonian of Eq. (2.15) reduces to a simple sum of independent one-body terms,

$$H_0 = -2 \sum_p \frac{d^2}{dB_p^2}; \quad -\pi \leq B_p \leq \pi, \quad (2.16)$$

each of which has two sets of eigenstates, namely $\{\cos mB; m = 0, 1, 2, \dots\}$ with even parity and $\{\sin mB; m = 1, 2, \dots\}$ with odd parity. The corresponding ground state is clearly a constant.

By analogy with the Néel model state for the spin-lattice problem discussed above, one can now take the ground state of the unperturbed Hamiltonian H_0 as our CCM model state $|\Phi\rangle$. Hence we have, $|\Phi\rangle = C$ with C a c-number. In the same spirit as before, one can define the n -body correlation operator S_n in terms of n -plaquette excitations with respect to this model state, and write the correlation operator S as

$$S = \sum_{k=1}^{N_p} S_k, \quad (2.17)$$

with

$$S_1 = \sum_{n=1}^{\infty} \sum_{p=1}^{N_p} S_p(n) \cos nB_p, \quad (2.18a)$$

$$S_2 = \frac{1}{2!} \sum_{n_1, n_2=1}^{\infty} \sum_{p_1, p_2=1}^{N_p} [S_{p_1 p_2}^{(1)}(n_1, n_2) \cos n_1 B_{p_1} \cos n_2 B_{p_2} + S_{p_1 p_2}^{(2)}(n_1, n_2) \sin n_1 B_{p_1} \sin n_2 B_{p_2}], \quad (2.18b)$$

where the prime on the summation excludes the terms with $p_1 = p_2$; and similarly for the higher-order partitions S_k with $k > 2$. We note also that such a definition of S is dictated by the requirement that the ground state, $|\Psi_g\rangle = \exp(S)|\Phi\rangle$, has even parity under the interchange of the sign of all variables $\{B_p\}$ simultaneously.

In order to derive the CCM coupled equations (2.5) and (2.6) one needs to define the inner product for the lattice gauge model. We define the inner product of two wave functions, $|f\rangle = |f(\{B_p\})\rangle$ and $|\bar{g}\rangle = |\bar{g}(\{B_p\})\rangle$, in the case of the $U(1)$ model, as

$$\langle \bar{g} | f \rangle = \int_{-\pi}^{\pi} \prod_{p=1}^{N_p} \left(\frac{dB_p}{2\pi} \right) \bar{g} \cdot f. \quad (2.19)$$

Thus $\langle \Phi | \Phi \rangle = 1$ if the constant value C is chosen to be unity.

The energy equation and the one-plaquette equations can be written together as

$$\langle \Phi | \cos n B_p e^{-S} H e^S | \Phi \rangle = E_g \delta_{n,0}; \quad n = 0, 1, 2, \dots, \quad (2.20)$$

and the two-plaquette equations consist of two sets of inner products,

$$\langle \Phi | \cos n_1 B_{p_1} \cos n_2 B_{p_2} e^{-S} H e^S | \Phi \rangle = 0, \quad (2.21a)$$

and

$$\langle \Phi | \sin n_1 B_{p_1} \sin n_2 B_{p_2} e^{-S} H e^S | \Phi \rangle = 0, \quad (2.21b)$$

where $n_1, n_2 = 1, 2, \dots$ and $p_1 \neq p_2$ as before.

Again one needs to employ a truncation scheme for any practical calculation in order to determine the coefficients $\{S_p(n)\}$, $\{S_{p_1 p_2}^{(i)}(n_1, n_2); i = 1, 2\}$, etc. As we shall see shortly, a local approximation which was developed for the spin-lattice problems also provides a very efficient approximation scheme for the lattice gauge models.

3. SPIN-LATTICE MODEL CALCULATIONS

As discussed in the previous section, the ground-state energy and ket-state coefficients for the XXZ spin-lattice Hamiltonian of Eq. (2.8) are determined by Eqs. (2.11) and (2.12) respectively. In this section we solve these coupled equations within several approximation schemes which have been developed and which have proved very successful in dealing with lattice problems in the course of our investigations [3]. In particular, we discuss in this article two approximation schemes, namely the so-called SUB n and LSUB m schemes. For a particular spin-1 chain employing a different Hamiltonian, we also make a similar CCM analysis using an alternative model state, which will be discussed in Sec. 3.3.

3.1 SUB n Scheme Based on the Néel Model State

The SUB n scheme is the most common truncation approximation of the CCM, in which one only keeps up to n -body correlations, i.e.

$$S \rightarrow S_{\text{SUB}n} = \sum_{k=1}^n S_k. \quad (3.1)$$

We have derived all equations within the SUB4 scheme for a general XXZ model [3]. Here we consider the SUB2 approximation based on the Néel model state as an example. As given by Eq. (2.11) the CCM coupled equations for the two-spin-flip coefficients are given by, with $S \rightarrow S_{\text{SUB2}} = S_2$,

$$\langle N2 | s_i^- s_j^+ e^{-S_2} H e^{S_2} | N2 \rangle = 0, \quad (3.2)$$

or, after some straightforward algebra,

$$\sum_{\rho} \left[(1 + 2\Delta b_1 + 2b_1^2) \delta_{\rho, r} - 4s(\Delta + 2b_1) b_r + 4s^2 \sum_{r'} b_{r'} b_{r-r'+\rho} \right] = 0, \quad (3.3)$$

where we have introduced the notation $b_r \equiv S_{i,j}$ with $r \equiv j - i$, taking advantage of the translational invariance of the lattice system. We note that in 1D r is simply an odd integer, but in 2D r is a lattice vector connecting a site on the A -sublattice with a site on the B -sublattice.

The full set of nonlinear SUB2 equations (3.3) can be solved analytically by a sublattice Fourier transform method [3]. The solution may be written for the 1D chain as

$$b_r = K \int_0^\pi \frac{dq}{\pi} \frac{\cos rq}{\cos q} (1 - \sqrt{1 - k^2 \cos^2 q}), \quad (3.4)$$

where

$$K \equiv \frac{1}{2s}(\Delta + 2b_1), \quad k^2 \equiv \frac{1 + 2\Delta b_1 + 2b_1^2}{(\Delta + 2b_1)^2}. \quad (3.5)$$

The coefficient b_1 is thus determined self-consistently by

$$b_1 = K \int_0^\pi \frac{dq}{\pi} (1 - \sqrt{1 - k^2 \cos^2 q}). \quad (3.6)$$

Once b_1 is determined, the ground-state energy is obtained from Eq. (2.11). For the isotropic spin- $\frac{1}{2}$ 1D model, i.e., $z = 2$ and $\Delta = 1$, we find $E_g/N \approx -0.4186$. This is in rather good agreement with the exact result of -0.4432 to the same accuracy of four significant figures.

More interestingly, the SUB2 solution given above predicts a phase transition which is given by the terminating point in Eq. (3.6), at which $k \rightarrow k_c = 1$, and beyond which Eq. (3.6) has no real solution. This terminating condition determines the critical anisotropy Δ_c , such that no real SUB2 solution exists for $\Delta < \Delta_c$. Numerical solution yields the values $\Delta_c \approx 0.3728$, 0.7985 and 0.8872 for the spin- $\frac{1}{2}$ models in 1D, 2D and 3D respectively. As discussed in detail [3], by the further calculation of spin-spin correlation functions, the staggered magnetization, and the low-lying excitations, this critical point corresponds to the known Ising-Heisenberg phase transition, which is known to occur at $\Delta = 1$ in 1D. (When the higher-order many-body correlations are included, our value of Δ_c moves closer to the exact value of 1 as expected [3].) Furthermore, at this critical point the SUB2 staggered magnetization is zero in 1D in agreement with the exact result [5], but *nonzero* in 2D and 3D. In particular, for the well-studied 2D spin- $\frac{1}{2}$ square lattice, this value is 0.682 in our SUB2 approximation,

Table 1. Ground-state energy per spin as a function of Δ for the 1D spin- $\frac{1}{2}$ XXZ model. Shown are the results of the LSUB n schemes with $n = 2, 4, 6, 8$, together with the exact results for comparison.

Method	Δ					
	0.0	0.5	1.0	1.5	2.0	5.0
LSUB2	-0.2887	-0.3412	-0.4167	-0.5069	-0.6076	-1.2986
LSUB4	-0.3193	-0.3692	-0.4363	-0.5195	-0.6155	-1.2995
LSUB6	-0.3198	-0.3730	-0.4400	-0.5218	-0.6167	-1.2995
LSUB8	-0.3196	-0.3741	-0.4414	-0.5226	-0.6170	-1.2995
Exact	-0.3183	-0.3750	-0.4432	-0.5234	-0.6172	-1.2995

in good agreement with the results of many other calculations including large-scale Monte Carlo simulations (and see references cited in Ref. [3]).

3.2 LSUB m Scheme Based on the Néel Model State

In the SUB2 scheme discussed above, one includes arbitrarily long-range correlations and hence it is possible to predict a phase transition. On the other hand, if one desires only to obtain the ground-state energy with high accuracy, there exists a very efficient alternative truncation scheme. This is a local approximation scheme, referred to as the LSUB m scheme, which takes advantage of the localized nature of the interactions on the lattice. Specifically, in a LSUB m approximation one retains only those local configurations in the correlation operator S specified by a nominal index m . In particular, for the spin-lattice models under consideration, the LSUB m scheme retains only those configurations which contain any number of spin flips with respect to the Néel model state over a region of m contiguous sites on the lattice, and which are compatible with the restriction of $s_{\text{total}}^z = 0$.

For example, we consider the case of $s = \frac{1}{2}$ in 1D. The LSUB2 scheme retains the single coefficient $b_1 = S_{i,i+1}$. Its determining equation can be derived from Eq. (3.3) as

$$1 - 2\Delta b_1 - 3b_1^2 = 0, \quad (3.7)$$

with solution $b_1 = (\sqrt{\Delta^2 + 3} - \Delta)/3$. Substituting in Eq. (2.11), one has $E_g/N = -5/12 \approx -0.4167$ for the isotropic case $\Delta = 1$. This is surprisingly close to the full SUB2 result of -0.4186 given previously.

In the LSUB4 scheme in 1D for the case of spin- $\frac{1}{2}$, one retains 3 independent coefficients, b_1 and $b_3 (\equiv S_{i,i+3})$ of the two-spin-flip configurations, and $g_4 (\equiv S_{i,i+2,i+1,i+3})$ of the first four-spin-flip configuration. The corresponding coupled equations are derived from Eq. (2.12) respectively as

$$1 - 2\Delta b_1 - 3b_1^2 + 2b_1 b_3 + 2b_3^2 + 2g_4 = 0, \quad (3.8a)$$

$$b_1^2 - 4\Delta b_3 - 4b_1 b_3 + g_4 = 0, \quad (3.8b)$$

$$-\Delta(b_1^2 + 2b_1 b_3) + g_4(\Delta + 4b_1 + b_3) + 2b_1 b_3^2 = 0. \quad (3.8c)$$



Figure 1. The nine independent configurations of the LSUB6 scheme for the 1D spin- $\frac{1}{2}$ model. The crosses indicate the flipped spins with respect to the Néel model state. Notice also that the three configurations in the first column constitute the LSUB4 scheme discussed in the text.

For the same 1D spin- $\frac{1}{2}$ chain the LSUB6 approximation retains 9 independent cluster correlation coefficients, with corresponding spin-flip configurations illustrated in Fig. 1 as an example. We have obtained numerical results for the ground-state energy in the LSUB m scheme with $m \leq 8$ for the 1D spin- $\frac{1}{2}$ model. In Table 1 we show the results for several values of Δ , together with the exact results for comparison. As can be seen from Table 1, one can obtain the ground-state energy with very high accuracy in this LSUB m scheme for relatively low levels of m , even for values of $\Delta < 1$ for which the perfect long-range ordering in the Néel state has been totally destroyed in the exact ground state.

3.3 Alternative Model States

So far we have considered the CCM analysis of spin-lattice systems based on the classical Néel state as our choice of model state. While this is a quite natural choice for the XXZ model which is likely to possess the Ising-like long-range order (at least for anisotropy in the range $\Delta \geq 1$), it may not be so for other spin-lattice systems since there may exist other phases for which different CCM model states may be more appropriate. (Indeed, this may also be true for the so-called critical phase of the XXZ model.)

In this section, we consider an interesting spin-1 model, namely, the 1D Heisenberg-biquadratic chain, which exhibits a particularly rich phase structure. The Hamiltonian of this model is given by

$$H = \sum_{l=1}^N [\cos \theta \mathbf{s}_l \cdot \mathbf{s}_{l+1} + \sin \theta (\mathbf{s}_l \cdot \mathbf{s}_{l+1})^2], \quad (3.9)$$

where $\mathbf{s}_l$ is a spin vector with $|\mathbf{s}_l| = 1$, and the coupling constants are expressed through the angular parameter θ . The antiferromagnetic region is given by $-\pi/4 < \theta < \pi/2$, with the remaining region being ferromagnetic. The pure Heisenberg model is given by $\theta = 0$.

There are some exact results [7-10] available for this Hamiltonian. Briefly, the system is integrable [8,10] using the Bethe ansatz [5] at both $\theta = -\pi/4$ and $\pi/4$.

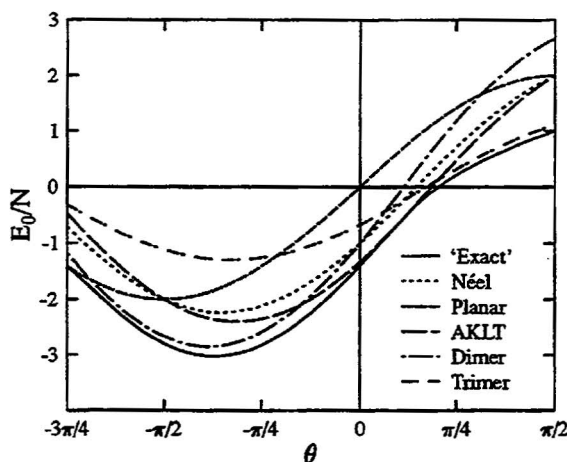


Figure 2. Expectation values of the spin-1 Hamiltonian of Eq. (3.9) with respect to several trial states as given by Eqs. (3.10). Also shown are the 'exact' results extrapolated from finite-size calculations (solid).

However, the corresponding periodicities in real space are two-fold and three-fold respectively. At $\theta = -\pi/2$ the system has been partially mapped [7] onto the spin- $\frac{1}{2}$ XXZ chain, and hence has been shown to have a nonzero gap and dimerization long-range order. At $\theta = \tan^{-1}(1/3)$, the exact ground state was shown by Affleck, Kennedy, Lieb and Tasaki [9] (AKLT) to be given by a uniform resonating valence bond configuration with no ordinary long-range order. The pure Heisenberg point, at $\theta = 0$, was discussed by Haldane who predicted the existence of a previously unexpected gap [6].

Based on these exact results and other analytical [11,12] and numerical [13] work, it seems reasonable to assume that there are at least three phases in the antiferromagnetic region, namely the homogeneous (or the AKLT-like [9]), dimerized, and trimerized phases. One possible additional phase, the 'spin-nematic' phase, has also been proposed by Chubukov [11] for θ near the ferromagnetic transition point at $\theta = -3\pi/4$.

In Fig. 2 we show the expectation values of Eq. (3.9) as functions of θ in various model states, namely, (i) the Néel state $|N2\rangle$ as discussed above; (ii) the so-called AKLT state [9], $|AKLT\rangle$, which is given by a simple valence-bond configuration with every atom connecting each of the two adjacent atoms by a valence bond; (iii) the dimerized (or spin-Peierls) state $|D\rangle$ which is given by a sequence of singlet states formed from pairs of adjacent atoms; (iv) the trimerized state $|T\rangle$ which is similar to the dimerized state but with each singlet state formed from three adjacent atoms; and finally (v) the planar state $|N1\rangle$ in which each atom has $s^z = 0$. These expectation values are given by the following expressions,

$$\langle N2|H|N2\rangle/N = -\cos\theta + 2\sin\theta, \quad (3.10a)$$

$$\langle AKLT|H|AKLT\rangle/N = -\frac{4}{3}\cos\theta + 2\sin\theta, \quad (3.10b)$$

$$\langle D|H|D\rangle/N = -\cos\theta + \frac{8}{3}\sin\theta, \quad (3.10c)$$

$$\langle T|H|T\rangle/N = -\frac{2}{3}\cos\theta + \frac{10}{9}\sin\theta, \quad (3.10d)$$

$$\langle N1|H|N1\rangle/N = 2\sin\theta. \quad (3.10e)$$

It is clear that the choice of model state with lowest energy depends critically on the value of θ . For example, near the ferromagnetic transition point at $\theta = -3\pi/4$, the planar model state has lowest energy; around $\theta = \tan^{-1}(1/3)$, the energy expectation value of the AKLT state is the lowest; while around $\theta > \pi/4$, the trimer state seems to give the lowest energy, etc. In any case, we now consider two CCM analyses for the Hamiltonian of Eq. (3.9), namely one based on the same Néel state as discussed above, and the other based on the new planar model state. We shall leave further discussion of other possible model states such as the trimerized or dimerized states to the final section.

(a) *A CCM analysis of the spin-1 chain based on the Néel model state*

The analysis of this case is the same as for the XXZ model except we use the Hamiltonian of Eq. (3.9) instead of that of Eq. (2.8). As an example we quote the result for the two-body coefficients $\{b_r\}$ in the full SUB2 approximation,

$$\sum_{\rho} [A\delta_{r,\rho} + Bb_r + C \sum_{r'} b_{r'} b_{r-r'+\rho}] = 0, \quad (3.11)$$

where $\rho = \pm 1$, where r, r' may be any positive or negative odd integers, and

$$A = -\cos\theta(1 + 2b_1 + 2b_1^2) + \sin\theta(1 + 2b_1)(1 + 2b_1 + 6b_1^2), \quad (3.12a)$$

$$B = 4\cos\theta(1 + 2b_1) - 4\sin\theta(1 + 4b_1 + 6b_1^2), \quad (3.12b)$$

$$C = -4\cos\theta + 4\sin\theta(1 + 2b_1). \quad (3.12c)$$

These equations can be solved in similar fashion to Eq. (3.3) by a Fourier transform technique. In Fig. 3 we show the SUB2 results from the solution of Eq. (3.11) for the ground-state energy as a function of θ . Interestingly, we observe again that there is a terminating point denoted as A, now at $\theta \approx 0.9864$, which is very close to the point $\theta = \pi/4$ where the exact results of Lai and Sutherland [10] reveal that the system has three-fold real space periodicity, in contrast to all the systems we have considered so far where the periodicity is two-fold. We therefore conclude that this terminating point may correspond to the critical point where the spin-1 system experiences a phase transition from a state like the model state $|N2\rangle$ with a two-fold periodicity to the state with a three-fold periodicity. The exact value of this critical point which separates the Haldane (AKLT simple valence-bond-like) phase from the trimerized phase is still not known, but it certainly lies in the range $\tan^{-1}(1/3) < \theta \leq \pi/4$.

(b) *A CCM analysis of the spin-1 chain based on the planar model state*

We now investigate the same Hamiltonian of Eq. (3.9) with a CCM analysis based on a different model state, namely the planar model state. By contrast with the Néel

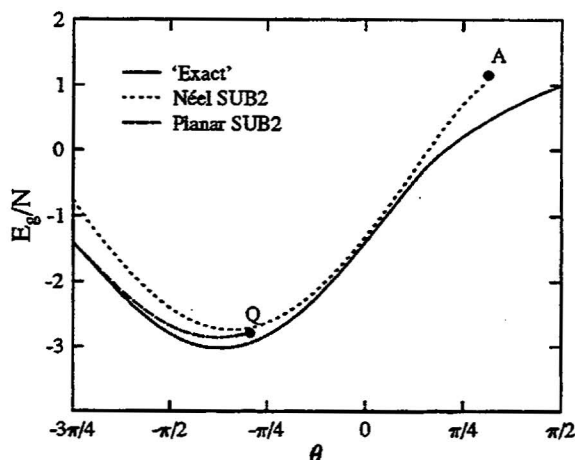


Figure 3. Ground-state energy per atom of the spin-1 Hamiltonian of Eq. (3.9) in the full SUB2 scheme, using the Néel model state and planar model state respectively. The 'exact' results extrapolated from finite-size calculations are also included for comparison.

model state, the planar model state $|N1\rangle$ is translationally invariant, and is given by the configuration with all spins in the $s^z = 0$ state,

$$|N1\rangle = |0, 0, 0, 0, 0, 0, 0, \dots\rangle. \quad (3.13)$$

The excitation operators with respect to $|N1\rangle$ clearly differ from those with respect to $|N2\rangle$. The usual raising and lowering operators $s_l^\pm$ cannot be used for a CCM analysis based on $|N1\rangle$. The reason is that to create a state on site l with $s^z = +1$ from $|N1\rangle$ one needs the operator s_l^+ , whereas to create a state with $s^z = -1$ requires s_l^- . Clearly s_l^- also acts as a destruction operator on the state with $s^z = 1$. Since the CCM correlation operator S is required from Eq. (2.3) to be composed only from creation operators this cannot be done using the $\{s_l^\pm\}$. In order to construct these new excitation operators for the planar model state of Eq. (3.13), we consider a single spin-1 atom which has the three states with $s^z = +1, 0, -1$, denoted as $|+\rangle, |0\rangle$, and $|-\rangle$ respectively. Therefore, using this basis $\{|+\rangle, |0\rangle, |-\rangle\}$, any spin operator can be expressed in terms of a 3×3 matrix which may be decomposed into a linear combination of 9 independent operators. We choose these as the 9 matrices each of which has 8 zero entries and a single nonzero entry which we take as 1 in each of the nine possible positions. Let A_{ij} be such a 3×3 matrix with 1 on the i th row and j th column (i.e., in a notation with $\langle i'|A_{ij}|j'\rangle = \delta_{ii'}\delta_{jj'}$, where $i, j = 1, 2, 3$ correspond respectively to the cases $s^z = +1, 0, -1$). We introduce new notations,

$$\begin{aligned} A_{11} &\equiv U^z; & A_{22} &\equiv C^z; & A_{33} &\equiv D^z; \\ A_{12} &\equiv U^+; & A_{32} &\equiv D^+; & A_{21} &\equiv U^-; & A_{23} &\equiv D^-; \\ A_{13} &\equiv U^m; & A_{31} &\equiv D^m. \end{aligned} \quad (3.14)$$

This notation is meant to suggest 'up', 'down', and 'centre', while the superscript m denotes 'maximal' (i.e., double '+' or double '-'). The algebra for these operators is simply given by

$$A_{ij}A_{kl} = A_{il}\delta_{jk}. \quad (3.15)$$

The Hamiltonian of Eq. (3.9) can then be written in terms of these operators. For example, the scalar product of two spin operators is given by

$$s_i \cdot s_j = (U_i^z - D_i^z)(U_j^z - D_j^z) + (U_i^+ + D_i^-)(U_j^- + D_j^+) + (U_i^- + D_i^+)(U_j^+ + D_j^-). \quad (3.16)$$

The excitation operators with respect to the planar model state of Eq. (3.13) are clearly given by the mutually commuting creation operators U^+ and D^+ . Therefore, the correlation operator S can now be constructed out of any combination of these two operators alone which is compatible with $s_{\text{total}}^z = 0$. In particular, $|\Psi_g\rangle$ is given in the SUB2 scheme based on the planar model state by,

$$|\Psi_g\rangle = e^S |N1\rangle, \quad S \rightarrow S_{\text{SUB2}} = \sum_{l=1}^N \sum_{\tau \neq 0} \beta_\tau U_l^+ D_{l+\tau}^+, \quad (3.17)$$

where τ runs over all (positive and negative) integers except zero.

The CCM energy equation analogous to Eq. (2.11) now reads,

$$\frac{E_g}{N} = 2\beta_1 \cos \theta + 2(1 - \beta_1) \sin \theta, \quad (3.18)$$

and the two-body equation is derived from

$$\langle N1 | U_l^- D_{l+\tau}^- \exp(-S_{\text{SUB2}}) H \exp(S_{\text{SUB2}}) | N1 \rangle = 0; \quad \tau = \pm 1, \pm 2, \dots, \quad (3.19)$$

or

$$\sum_{\rho} \left[K_1 \delta_{\rho, \tau} + K_2 \beta_\tau + K_3 \beta_{\tau+\rho} + K_4 \sum_{\tau' \neq 0} \beta_{\tau'} \beta_{\tau' - \tau + \rho} \right] = 0, \quad (3.20)$$

with $\beta_0 = 0$, and where

$$K_1 \equiv (1 - \beta_1 + 3\beta_1^2) \cos \theta - (1 - 3\beta_1 + 3\beta_1^2) \sin \theta, \quad (3.21a)$$

$$K_2 \equiv -6\beta_1 \cos \theta - 2(1 - 3\beta_1) \sin \theta, \quad (3.21b)$$

$$K_3 \equiv 2 \cos \theta, \quad (3.21c)$$

$$K_4 \equiv \cos \theta - \sin \theta. \quad (3.21d)$$

In these equations $\rho = \pm 1$, and τ, τ' run over all nonzero integers.

Again the solution of the SUB2 equation can be found by a Fourier transform technique and numerical results are also shown in Fig. 3. There are two terminating points in this case. One is located exactly at $\theta = -3\pi/4$ at which $\beta_1 = 0$ and $E_g/N = -\sqrt{2}$, and the other, denoted as Q, is at $\theta \approx -0.9209$ at which $\beta_1 \approx -0.4264$ and $E_g/N \approx -2.7874$. We note that the system becomes ferromagnetic at the first of these terminating points. The terminating point Q is more interesting. It lies rather

close in energy to the Néel SUB2 solution given above. In fact, the results of the LSUB2 approximations in which only the single coefficient b_1 or β_1 is retained using the Néel and planar model states respectively, cross at $\theta \approx -0.9050$ which is very close to the point Q. Such crossings are very commonly regarded in many-body theory as evidence of a phase change. The fact that the CCM full SUB2 approximation based on the planar model state terminates here is additional evidence for such a phase change. We note that in the absence of correlations the estimates $\langle N2|H|N2 \rangle$ and $\langle N1|H|N1 \rangle$ for the ground-state energy from Eq. (3.10a) and (3.10e) cross at the point $\theta = -\pi/2$ (and $+\pi/2$). By contrast, when the correlations in both LSUB2 approximations based on the Néel and planar states are included, the crossover occurs much closer to the point $\theta = -\pi/4$ at which the phase transition occurs between the two-fold degenerate dimerized phase (which exists for $-3\pi/4 < \theta < -\pi/4$) and the nondegenerate Haldane (AKLT valence-bond) phase.

4. $U(1)$ LATTICE GAUGE MODEL CALCULATIONS

The model state $|\Phi\rangle$ and the correlation operator S for the $U(1)$ model Hamiltonian of Eq. (2.15) have been discussed in Sec. 2.3. Here we present the results of calculations based on this analysis.

4.1 One-Plaquette Approximation

The one-plaquette coefficients $\{S_p(n)\}$ are determined, within the SUB1 approximation, by Eq. (2.20) with the substitution

$$S \rightarrow S_{\text{SUB1}} = S_1, \quad (4.1)$$

where the one-plaquette correlation operator S_1 is given by Eq. (2.18a). In our previous work [4] we have published the results of this SUB1 scheme. We therefore will not discuss them again except to quote the equation and define a subtruncation scheme which will be employed again for the SUB2 scheme discussed later. After an extension of the definition for $\{S_p(n)\}$ to include the negative modes (negative n), and taking advantage of the lattice translational invariance to introduce the definition

$$a_m \equiv mS_p(m); \text{ with } a_m = -a_{-m}, \text{ and } a_0 = 0, \quad (4.2)$$

Eq. (2.20) can then be readily written as

$$\left(\frac{E_g}{N_p} - \lambda\right) \delta_{m,0} + \frac{1}{2}\lambda(\delta_{m,1} + \delta_{m,-1}) - ma_m - \frac{1}{2} \sum_{n=-\infty}^{\infty} a_n a_{m-n} = 0, \quad (4.3)$$

where m may be any integer. We note that the energy equation is given by setting $m = 0$. Equation (4.3) can in fact be transformed to the well-known Mathieu equation corresponding to the single-body Schrödinger equation with the one-plaquette Hamiltonian given by the first term of Eq. (2.15) [4].

We solve these SUB1 equations numerically by a hierarchical sub-truncation scheme, the so-called SUB1(n) scheme in which one retains at the n th level of approximation only those coefficients a_m with $|m| \leq n$, and sets the remainder with $|m| > n$

to zero. For example, in the SUB1(1) scheme, a_1 is the only retained coefficient. The solution is trivially obtained from Eq. (4.3) as

$$a_1 = \frac{\lambda}{2}, \quad \frac{E_g}{N_p} = \lambda - \frac{1}{4}\lambda^2; \quad \text{SUB1(1)}. \quad (4.4)$$

This SUB1(1) result is in fact identical to the result obtained from the second-order perturbation theory about the strong-coupling ($\lambda \rightarrow 0$) limit. However, the subsequent SUB1(n) approximations with $n > 1$ give results far superior to those of perturbation theory. A detailed discussion has been given in Ref. [4].

4.2 Two-Plaquette Approximation

We next discuss the two-plaquette approximation, i.e., the SUB2 scheme in which one makes the substitution

$$S \rightarrow S_{\text{SUB2}} = S_1 + S_2. \quad (4.5)$$

As defined by Eq. (2.18b), there are two sets of two-plaquette coefficients which are determined by Eqs. (2.21a) and (2.21b) respectively. Together with the one-plaquette equations discussed above, one has three sets of coupled equations. Obviously these full SUB2 equations are quite involved because there exist mode couplings in addition to the plaquette correlations. This is different from the SUB2 scheme for the spin-lattice models considered in Sec. 3 where only the spin-spin correlations exist.

Fortunately, as is well known [14], the local fluctuations in the lattice gauge theory dominate, and one does not expect a phase transition, at least for the 1D and 2D $U(1)$ models. We therefore employ our local approximation developed for the spin-lattice models, namely the LSUB m scheme, to calculate the ground-state energy with the correlation effects included. We shall discuss the LSUB2 scheme which includes only the nearest-neighbour plaquette correlations. (We have also referred to this LSUB2 scheme as the SUB2-1 approximation in the literature [4].) We need first to simplify our notations for the two-plaquette coefficients. Using the lattice symmetry properties, one can write

$$S_{p_1 p_2}^{(1)}(n_1, n_2) \equiv b_r(n_1, n_2), \quad S_{p_1 p_2}^{(2)}(n_1, n_2) \equiv c_r(n_1, n_2), \quad r \equiv p_2 - p_1. \quad (4.6)$$

Clearly, r is simply an integer for the 1D array of plaquettes, but a lattice vector of the square lattice for the 2D case. The LSUB2 approximation retains those coefficients $b_r(n_1, n_2)$ and $c_r(n_1, n_2)$ with $|r| = 1$ only.

Similar to the SUB1(n) scheme discussed above, we may also introduce the so-called LSUB2(n) sub-truncation scheme to incorporate the mode-mode couplings systematically. For example, the LSUB2(1) scheme is identical to the SUB1(1) scheme considered previously in which only a single coefficient a_1 is retained. In the LSUB2(2) scheme, however, four coefficients are retained. They are a_1 and a_2 from the one-plaquette equations, and $b_1(1, 1)$ and $c_1(1, 1)$ from the two-plaquette correlations. The corresponding equations, together with the energy equation, are given in this local 2-mode approximation by,

$$\frac{E_g}{N_p} = \lambda - a_1^2 - a_2^2 - \frac{z}{4}b_1c_1 - \frac{z}{2}(b_1^2 + c_1^2); \quad (4.7a)$$

$$-\frac{\lambda}{2} + a_1 - a_1 a_2 - z a_1 \left(b_1 + \frac{1}{4} c_1 \right) = 0; \quad (4.7b)$$

$$2a_2 + \frac{1}{2} a_1^2 = 0; \quad (4.7c)$$

$$(1 - a_2) \left(b_1 + \frac{1}{4} c_1 \right) = 0; \quad (4.7d)$$

$$\frac{1}{4} a_1^2 + (1 + a_2) \left(\frac{1}{4} b_1 + c_1 \right) = 0; \quad (4.7e)$$

where we have simplified the notation further by writing $b_1 \equiv b_1(1, 1)$ and $c_1 \equiv c_1(1, 1)$, and where z is again the lattice coordination number (i.e., $z = 2$ for the 1D chain and $z = 4$ for the 2D lattice). In the strong-coupling limit ($\lambda \rightarrow 0$) this LSUB2(2) approximation exactly reproduces the results of the corresponding perturbation series up to the fourth order,

$$\frac{E_g}{N_p} \xrightarrow{\lambda \rightarrow 0} \begin{cases} \lambda - \frac{1}{4} \lambda^2 + \frac{89}{3840} \lambda^4 + O(\lambda^6), & 1D; \\ \lambda - \frac{1}{4} \lambda^2 + \frac{73}{3840} \lambda^4 + O(\lambda^6), & 2D. \end{cases} \quad (4.8)$$

We have also derived and solved the LSUB2(n) equations up to $n = 10$. For example, the LSUB2(3) scheme retains 7 independent coefficients. In addition to the four coefficients of the LSUB2(2) scheme discussed, the three additional coefficients are $a_3, b_1(1, 2)$ ($= b_1(2, 1)$) and $c_1(1, 2)$ ($= c_1(2, 1)$). Generally, there are N_n independent coefficients within the LSUB2(n) scheme, where N_n is given by

$$N_n = \left[n \left(\frac{1}{2} n + 1 \right) \right], \quad (4.9)$$

and where the symbol $[A]$ denotes the integer part of the number A .

The results for the ground-state energy in the LSUB2(n) scheme up to $n = 10$ are shown as functions of λ in Table 2 and Fig. 4, together with some results of strong-coupling perturbation theory. In Table 2 we have also included the results from the method of correlated basis functions (CBF) [15], and from an analytical continuation of the strong-coupling perturbation series [16]. Our LSUB2(10) results are in good agreement with them. One sees clearly in Fig. 4 that our LSUB2(n) results quickly converge as n increases. It is also clear that the perturbation series gives very poor results for $\lambda \geq 1.5$, a value which seems to be a good estimate for its radius of convergence. Much work in modern field theory goes into attempts to analytically continue such perturbation series as Eq. (4.8) outside their natural boundaries. A typical recent such attempt [16] for the 2D $U(1)$ model starts from the strong-coupling perturbation series of Eq. (4.8), utilizing the known coefficients up to $O(\lambda^{18})$ as input to generalized Padé approximants. We should emphasize that our own LSUB2(n) approximations themselves represent a natural extension of perturbation theory. They comprise, in effect, a well-defined analytic continuation or resummation of the perturbation theory results within the context of a natural and consistent hierarchy of approximations. They may be contrasted with the rather *ad hoc* approaches based on Padé and other

Table 2. Ground-state energy per plaquette at several values of λ for the 2D $U(1)$ model. Shown are the results of the LSUB2(n) schemes with $n = 2, 3, 4, 5, 6, 8, 10$, together with the full SUB1 results and the results of both strong ($\lambda \rightarrow 0$) and weak ($\lambda \rightarrow \infty$) coupling limits in perturbation theory. We show the results of fourth- and eighth-order strong-coupling perturbation theory, PT4(S) [and see Eq. (4.8)] and PT8(S) respectively, and of lowest-order weak-coupling perturbation theory, PT(W) [and see Eq. (4.10)]. The results from the correlated basis function (CBF) approach of Dabringhaus, Ristig and Clark [15], and from an analytic continuation of the strong-coupling perturbation series by Hamer, Oitmaa, and Zheng [16], denoted as HOZ, are also included for comparison purposes.

Method	λ								
	0.5	1	2	3	4	5	6	8	10
SUB1	0.4391	0.7724	1.2430	1.5828	1.8597	2.1000	2.3156	2.6966	3.0315
LSUB2(2)	0.4386	0.7652	1.1468	1.1280	0.3019	-2.833	-15.11	-	-
LSUB2(3)	0.4387	0.7681	1.2216	1.5371	1.7691	1.9282	2.0153	1.9720	1.6422
LSUB2(4)	0.4387	0.7681	1.2214	1.5428	1.7994	2.0123	2.1921	2.4585	2.6365
LSUB2(5)	0.4387	0.7681	1.2216	1.5442	1.8043	2.0237	2.2105	2.4977	2.6753
LSUB2(6)	0.4387	0.7681	1.2217	1.5453	1.8099	2.0404	2.2482	2.6188	2.9512
LSUB2(8)	0.4387	0.7681	1.2217	1.5454	1.8100	2.0404	2.2477	2.6142	2.9358
LSUB2(10)	0.4387	0.7681	1.2216	1.5452	1.8095	2.0393	2.2456	2.6096	2.9278
CBF	0.4387	0.7677	1.2167	1.5335	1.7929	2.0201	2.2255	-	-
PT4(S)	0.4387	0.7690	1.3042	2.2898	4.8667	10.632	21.638	-	-
PT8(S)	0.4387	0.7673	1.1358	-0.738	-20.87	-	-	-	-
HOZ	-	-	1.215	-	1.785	-	2.2	-	-
PT(W)	0.5627	0.8434	1.2402	1.5447	1.8015	2.0276	2.2321	2.5917	2.9150

resummation techniques, which usually find it difficult to approach the weak-coupling limit with the correct asymptotic form unless this is built in from the start.

It is worth mentioning that in quantum chemistry and other many-body systems, the more relevant physical quantity is the so called correlation energy which is defined as the difference between the mean-field one-body (SUB1 in the present case) and the exact ground-state energies. This correlation energy can be measured experimentally in the cases of atoms and molecules. From Fig. 4 and Table 2, one can see that the correlation energy within the LSUB2 approximation (i.e., the LSUB2 results minus the SUB1 results) in the $U(1)$ model is quite small, and much smaller than the total energy. We suspect that this is true for lattice gauge field theories in general. This is quite similar to the case in quantum chemistry where the correlation energy is typically only a few percent at most of the total energy. It is clear that a powerful many-body technique is required in order to obtain a sensible numerical value for this correlation energy.

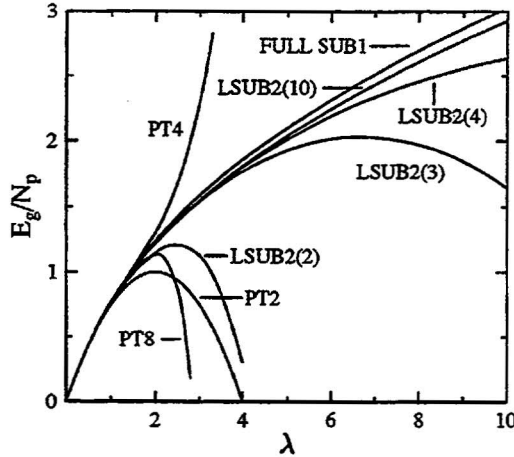


Figure 4. Ground-state energy per plaquette for the 2D $U(1)$ model on the square lattice in the LSUB2(n) scheme with $n = 2, 3, 4, 10$. Also shown are the full SUB1 results and the results from the n th-order strong-coupling perturbation series, PT n , with $n = 2, 4, 8$.

We should also point out that one cannot reproduce, from our LSUB2(n) equations, the correct coefficients of the perturbation series in the weak-coupling limit ($\lambda \rightarrow \infty$), which is given by

$$\frac{E_g}{N_p} \xrightarrow{\lambda \rightarrow \infty} C_0 \sqrt{\lambda} - \frac{1}{8} C_0^2 + O(\lambda^{-1/2}), \quad (4.10)$$

where $C_0 = 1, 0.9833, 0.9581$ in 0D (i.e., one-plaquette or Mathieu problem), 1D and 2D respectively, although our LSUB2(n) schemes do give good results even for very large values of λ , as can be seen from Table 2 and Fig. 4. Some results from the first two terms of weak-coupling perturbation series of Eq. (4.10) have also been included in Table 2 for comparison, where they are denoted as PT(W). However, by employing a different model state, one can reproduce *both* the correct strong- and weak-coupling limits as we shall discuss next.

4.3 Alternative Mean-Field-Like Model State

In the above CCM calculations, the model state $|\Phi\rangle$ was chosen as the ground-state wavefunction of the strong-coupling limit Hamiltonian of Eq. (2.16), i.e., a constant. This is certainly not the only choice. For example, one can take a mean-field-like wavefunction as our CCM model state. In fact, CCM calculations based on a mean-field-like model state, sometimes referred to as the maximum-overlap criterion, have been carried out for the ϕ^4 field theory and other many-body problems [17].

In the current context, the mean-field-like wavefunction self-consistently includes one-plaquette correlations and can be written as,

$$|\Phi_{mf}\rangle = \exp(T)|\Phi\rangle, \quad (4.11)$$

where $|\Phi\rangle$ is, as before, the constant ground-state wavefunction of H_0 and where T can be expressed in lowest order in terms of the single one-plaquette variable,

$$T \equiv \frac{1}{2} t \sum_{p=1}^{N_p} \cos B_p, \quad (4.12)$$

with t a parameter yet to be determined. A simple energy minimization can be carried out by treating t as a variational parameter in the expectation value of the Hamiltonian with respect to this $|\Phi_{mf}\rangle$, namely

$$\frac{d}{dt} \langle H \rangle = 0, \quad \text{with} \quad \langle H \rangle \equiv \frac{\langle \Phi_{mf} | H | \Phi_{mf} \rangle}{\langle \Phi_{mf} | \Phi_{mf} \rangle}. \quad (4.13)$$

A straightforward evaluation yields the result,

$$\frac{\lambda}{t} I_0(t) I_1(t) + \left(\frac{t}{2} - \lambda \right) (I_0^2(t) - I_1^2(t)) = 0, \quad (4.14)$$

where $I_n(x)$ is the modified Bessel function of order n ,

$$\frac{1}{\pi} \int_0^\pi d\theta \cos n\theta \exp(x \cos \theta) = I_n(x). \quad (4.15)$$

The solution of Eq. (4.14) for t leads to the correct leading-order perturbation series terms for the ground-state energy in both strong- and weak-coupling limits,

$$\frac{\langle H \rangle}{N_p} = \lambda + \left(\frac{t}{2} - \lambda \right) \frac{I_1(t)}{I_0(t)} = \begin{cases} \lambda - \frac{1}{4} \lambda^2 + O(\lambda^4), & \text{for } \lambda \rightarrow 0; \\ \sqrt{\lambda} - \frac{1}{8} + O(\lambda^{-1/2}), & \text{for } \lambda \rightarrow \infty. \end{cases} \quad (4.16)$$

More precisely, this (variational) mean-field calculation reproduces the result of lowest-order strong-coupling perturbation theory in all dimensions, since this result is itself independent of the coordination number of the lattice, whereas it reproduces the exact weak-coupling limit only of the (zero-dimensional) single-plaquette case. Nevertheless, as we have indicated in our discussion below Eq. (4.10), the weak-coupling limits for the 1D chain and 2D square lattice are themselves very close to that of the single-plaquette Mathieu problem.

Hence, one can now carry out similar CCM calculations as discussed above, but based on $|\Phi_{mf}\rangle$ as model state instead of the constant $|\Phi\rangle$. The only change is that in each inner product as in Eqs. (2.20) - (2.21), for example, one replaces the constant model state $|\Phi\rangle$ by the mean-field-like model state $|\Phi_{mf}\rangle$. We expect such calculations to produce results which are correct in both the strong- and weak-coupling limits, and hence rather accurate over the entire range of λ . We are currently carrying out such calculations and will report our results in the near future.

5. INTRODUCTION TO A CCM ANALYSIS FOR THE $SU(2)$ MODEL

The Hamiltonian of a general non-Abelian lattice gauge field theory is given, in the case of pure gauge without quark fields, by

$$H = \frac{1}{2} \sum_l E_l^\alpha E_l^\alpha + \lambda \sum_p (1 - \cos B_p), \quad (5.1)$$

where, like the Abelian gauge model of Eq. (2.11), the first sum is over all links l while the second is over all plaquettes p . But, different from the Abelian case, the electric field E_l ($\equiv E_l^\alpha$) here is a vector and in Eq. (5.1) the convention of two repeated indices implying the summation over the corresponding index is assumed. In particular, for the $SU(2)$ model under consideration, E^α is a three-dimensional vector (with $\alpha = x, y, z$). The magnitude B_p of the magnetic field vector B_p is defined by the trace of the product of four members of the $SU(2)$ group defined on the links of the plaquette p as

$$\cos B_p \equiv \frac{1}{2} \text{Tr } U_p, \quad \text{with } U_p = U_1 U_2 U_3^{-1} U_4^{-1}, \quad (5.2)$$

where the link variable U_l is defined through the vector potential A_l as

$$U_l \equiv \exp \left(\frac{1}{2} i \sigma^\alpha A_l^\alpha \right), \quad (5.3)$$

with σ^α the usual Pauli matrices that form the generators of the $SU(2)$ algebra.

The basic algebra for the $SU(2)$ model is given by the following commutation relation,

$$[E_l^\alpha, U_l] = \frac{1}{2} \delta_{ll'} \sigma^\alpha U_l. \quad (5.4)$$

In view of the successful application of the CCM to the Abelian $U(1)$ lattice gauge model discussed in Sec. 4, we intend to apply a similar CCM analysis to this non-Abelian $SU(2)$ model. As one may notice immediately, the first main difference between the $SU(2)$ and $U(1)$ models lies in the fact that both the electric field E_l and the magnetic field B_p are three-dimensional vectors in the $SU(2)$ model, whereas they are scalars in the $U(1)$ model. The fact that both E_l and B_p are vectors in the $SU(2)$ model implies that one has to include the angular dependences in the two-body (and higher-order) correlation operator S_2 given by the counterpart to Eq. (2.18b). Although this work is still in progress, it is clear that for the case of the one-plaquette problem, similar calculations to those in Sec. 4.1 can be carried out for the $SU(2)$ model with only minor modifications.

Specifically, we still choose a constant wavefunction for our model state $|\Phi\rangle$, and write the one-plaquette correlation operator S_1 as

$$S_1 = \sum_{n=1}^{\infty} S(n) \cos nB, \quad (5.5)$$

where we have suppressed the plaquette index p because we consider only the case of the one-plaquette problem for the moment. The energy and one-plaquette equations are similar to Eq. (2.20), but the inner product between a ket state $|f\rangle$ and a bra state $\langle \tilde{g}|$ is now defined by

$$\langle \tilde{g}|f\rangle = \frac{1}{\pi} \int_0^{2\pi} \tilde{g} \cdot f \sin^2 B dB, \quad (5.6)$$

where the new integration measure, $\frac{1}{\pi} \sin^2 B dB$, reflects the fact that B is the magnitude of a vector.

Equation (2.20) for the case of the one-plaquette $SU(2)$ model then becomes, with $e_0 \equiv E_g$,

$$\begin{aligned} (e_0 - \lambda) \left[\delta_{n,0} - \frac{1}{2}(\delta_{n,2} + \delta_{n,-2}) \right] + \frac{1}{4} \lambda (\delta_{n,1} + \delta_{n,-1} - \delta_{n,3} - \delta_{n,-3}) \\ - \frac{1}{4} \left[n a_n - \frac{1}{2}(n+2)a_{n+2} - \frac{1}{2}(n-2)a_{n-2} \right] - \frac{1}{4}(a_{n+2} - a_{n-2}) \\ + \frac{1}{8} \sum_{m=-\infty}^{\infty} a_m \left(a_{m-n} - \frac{1}{2}a_{m-n-2} - \frac{1}{2}a_{m-n+2} \right) = 0, \end{aligned} \quad (5.7)$$

where, as before in Eq. (4.2), we have extended the definition of the one-plaquette coefficients $a_n \equiv nS(n)$ to include the negative modes. This equation similarly arises for the N_p -plaquette $SU(2)$ model in the SUB1 approximation, with $e_0 \rightarrow E_g/N_p$. Equation (5.7) can in fact again be transformed into the well-known antisymmetric Mathieu equation which characterizes the $SU(2)$ single-plaquette problem by first making a Fourier transform,

$$A(B) = \sum_{m=-\infty}^{\infty} a_m \sin mB, \quad (5.8)$$

and then by making the familiar Riccati transform $A(B) = -2\psi'(B)/\psi(B)$. We thus readily find,

$$-\frac{1}{2} \sin B \psi'' - \cos B \psi' + \lambda(1 - \cos B) \sin B \psi = e_0 \sin B \psi. \quad (5.9)$$

Finally, by making the substitution $\phi = \sin B \psi$, one derives the following Mathieu equation,

$$\left[-\frac{1}{2} \left(\frac{d^2}{dB^2} + 1 \right) + \lambda(1 - \cos B) \right] \phi(B) = e_0 \phi(B), \quad (5.10)$$

where we now seek the lowest antisymmetric solution [18]. It is not difficult to perform the similar calculations of the SUB1(n) scheme, as discussed in Sec. 4.1, for Eq. (5.7). We do not therefore go into detail here.

6. DISCUSSION AND EXTENSIONS

In this article we have reviewed our applications of the CCM to the two archetypal Hamiltonian lattice problems, namely the spin-lattice systems and the Abelian lattice gauge field models. The emphasis has been placed on the systematic, unified approximation schemes developed in the course of our investigation for obtaining with high accuracy the ground-state energy and such other physical quantities as the excitation energy and long-range order parameter.

The results presented in this article convince us that the extension of the current approach to other Hamiltonian lattice systems of interest is a natural and urgent next step. One such lattice system is the electronic Hubbard and allied models which, despite intensive studies by various theoretical techniques, are still not well-understood.

We notice that some preliminary attempts have been made in this direction [19]. The extension of our calculations for the $U(1)$ lattice gauge model in this paper to such other non-Abelian lattice gauge models as the $SU(2)$ model is also well under way. We are interested, furthermore, to carry out similar CCM calculations for the low-dimensional spin-lattice systems, e.g., the spin-1 Heisenberg-biquadratic chain of Eq. (3.9), and other interesting spin- $\frac{1}{2}$ chains with nearest- and next-nearest-neighbour couplings, but using the dimerized or trimerized valence-bond states of the types discussed in Sec. 3.3 as our model states. We hope to report the results of all these calculations in the near future.

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