Series Expansions for Excited States of Quantum Lattice Models

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Abstract

We show that by means of connected-graph expansions one can effectively generate exact high-order series expansions which are informative of low-lying excited states for quantum many-body systems defined on a lattice. In particular, the Fourier series coefficients of elementary excitation spectra are directly obtained. The numerical calculations involved are straightforward extensions of those which have already been used to calculate series expansions for ground-state correlations and $T = 0$ susceptibilities in a wide variety of models. As a test, we have reproduced the known elementary excitation spectrum of the transverse-field Ising chain in its disordered phase.

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Several years ago, Singh, Huse and this author [1,2] described an efficient, general method for calculating high-order perturbations expansions for ground-state correlations and $T = 0$ susceptibilities in quantum many-body systems defined on a lattice. (It is worth noting, belatedly, that we rediscovered methods that had been developed first by Hamer, Nickel, and others; a convenient entry point into that literature is He et al. [3].) This method had two principle facets: (1) A connected-cluster (a.k.a. “linked-cluster”, “connected-graph”, or simply “cluster”) expansion for the properties of interest, combined with (2) a formulation of Rayleigh-Schrödinger perturbation theory in terms of a recurrence relation, for the purpose of constructing the ground state energy and eigenvector perturbatively on each cluster. This method has been applied to a wide variety of problems involving $S = 1/2$ and $S = 1$ antiferromagnets [4] and also to the Kondo lattice model of mobile fermions and stationary spins [5]. In every case one considers a family of Hamiltonians parameterized by $\lambda$,

$$H = H_0 + \lambda H_1,$$

in which the “unperturbed” Hamiltonian is trivially diagonalizable and of fixed degeneracy on any connected cluster of sites.

The perturbation expansion approach is comparable in many respects to finite-size diagonalization studies. A major advantage of the former is that the series expansions do not suffer from finite-size and shape effects — they are exact for the infinite lattice. A major disadvantage has been that many important properties associated with excited states, such as elementary excitation spectra and their associated residues, were inaccessible. Here I show that these properties can be calculated in terms of perturbation expansions about trivial unperturbed Hamiltonians, by direct (but hardly obvious, a priori) extensions of the two crucial facets of the method for ground state properties which are listed above. The algorithms are simple in principle, and if computer code for generating the ground-state series expansions for some model already exists then it is straightforward to modify it so as to yield excited-state data.

The key to the approach is to construct the effective Hamiltonian within a degenerate
(for $H_0$) manifold of excited states for each finite cluster. The formulae which yield perturbation expansions for the effective Hamiltonians are derived by considering a similarity transformation

\[ S^{-1}HS = H^{\text{eff}} \]

where $H$ is the Hamiltonian restricted to some finite cluster, and written explicitly in the basis of the eigenstates of $H_0$. For definiteness we assume there are $L$ degenerate states out of $M$ states total, and it is useful to order the eigenstates of $H_0$ so that the first $L$ are those of the manifold. We can choose $S$ so as to not mix the states within the degenerate manifold, that is, we take it to be the identity within the upper left $L \times L$ block. The matrix $S$ is to be constructed so that in $H^{\text{eff}}$ there are vanishing matrix elements between the degenerate manifold and the other states, that is, $H^{\text{eff}}$ breaks up onto an $L \times L$ block in the upper left, describing the interactions between the “dressed” states of the manifold, and an $(M - L) \times (M - L)$ block, describing all the other (irrelevant) physics of the cluster. Traditionally (for example, the Foldy-Wouthuysen transformation of the Dirac equation), $S$ would be written as $e^{iT}$ and the Hermitian operator $T$ written as a power series in $\lambda$, the exponentials would be expanded, and the vanishing of the appropriate $H^{\text{eff}}$ matrix elements would lead to a set of equations for the terms in the series for $T$. Rather than expanding exponentials, we construct $H^{\text{eff}}$ simply by moving $S^{-1}$ to the other side and viewing $S$ as a set of column vectors $\psi^{(l)}$. We now have an equation in which the vectors $\psi^{(l)}$ with $1 \leq l \leq L$ are not coupled to those with $L + 1 \leq l \leq M$, and we can now entirely neglect the part of $H^{\text{eff}}$ that lies outside the $L \times L$ block. Then expand everything in sight in powers of $\lambda$:

\[ \psi^{(l)} = \sum_k \lambda^k \psi^{(l)}_k, \]

\[ H^{\text{eff}}(l', l) = \sum_k \lambda^k H^{\text{eff}}_k(l', l) \]

and collect the terms proportional to $\lambda^k$ in column $l$ to yield

\[ H_0 \psi^{(l)}_k + H_1 \psi^{(l)}_{k-1} = \sum_{k'=0}^L \sum_{l'=1}^M \psi^{(l')}_{k'} H^{\text{eff}}_{k-k'}(l', l). \]
From this equation one can now almost immediately write coupled recurrence relations for the terms in the power series expansions of $H_{\text{eff}}$ and the $\psi^{(l)}$. It is only necessary to impose a “normalization convention” (which affects the form of the final equations but not any of the physical results): it is most convenient to require for states $|l\rangle$ in the degenerate manifold of $H_0$ that

$$
\langle l|\psi^{(l')}\rangle = \delta_{k,0}\delta_{l,l'}.
$$

Then one has for the effective Hamiltonian

$$
H_{\text{eff}}^{(m,l)} = \langle m|H_1|\psi^{(l)}\rangle_k - \langle m|H_1|\psi^{(l)}\rangle_{k-1},
$$

and for the projection of $|\psi^{(l)}\rangle$ onto an eigenstate state of $H_0$ outside the manifold the result is

$$
\langle n|\psi^{(l)}\rangle = \frac{1}{E_0 - E_n} \left( \langle n|H_1|\psi^{(l)}\rangle_k - \sum_{k'=1}^{k-1} \sum_{l'=1}^{L} H_{\text{eff}}^{(k-k',l,l')} \langle n|\psi^{(l')}\rangle \right).
$$

where $E_0$ is the unperturbed energy of the states in the degenerate manifold and $E_n = \langle n|H_0|n\rangle$. These last two equations are the desired recurrence relations.

The next problem to address is how to carry out subgraph subtraction, so that one can obtain an exact $n$th order expansion by considering only a finite number of connected clusters. (See for example Ref. [2] for a general discussion of subgraph subtraction, which is at the heart of the cluster expansion approach to constructing series expansions.) But at the moment, it is not entirely obvious what quantities one is supposed to be subtracting! The point one has to establish is that weight of the quantity $Q$ under consideration vanishes for a disconnected graph; or, equivalently, for a graph $C$ consisting of two unconnected clusters $A$ and $B$, $Q_C = Q_A + Q_B$.

Since we are going to have to discuss specific quantities it is advantageous to consider a specific model, and for the sake of clarity we choose a particularly simple one: the $S = 1/2$ transverse-field Ising model defined by

$$
H = -\sum_i \sigma_i^z - \lambda \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x.
$$
We will consider a “disordered state” expansion, in which $H_0$ is the first term and $H_1$ the second term (except for the factor $\lambda$). Although the explicit discussion in the next several paragraphs will be concerned entirely with this model, it should be fairly clear that other models (such as the Kondo lattice model, variants of the $t$-$J$ model, the Heisenberg-Ising model, and other models for which the ground-state properties have been studied by means of series expansions) may be treated along similar lines.

For any $N$-site cluster the ground state of $H_0$ is the unique state with $\sigma_{\text{tot}}^z = N$, namely, $\left| \uparrow \ldots (N \text{ times}) \uparrow \right\rangle$. The lowest excited states form an $N$-fold degenerate set, the most natural basis set being $\left| \downarrow \uparrow \ldots (N - 1 \text{ times}) \uparrow \right\rangle$, etc. One can label these “single-flipped-spin” states by the site of the cluster which carries the flipped spin. In the thermodynamic limit, one could equally well say that $H_0$ has a dispersionless mode with energy 2. We will now proceed to show how one can use perturbation theory to determine how this spectrum evolves as the Ising coupling is turned on.

Suppose we have a cluster $C$ with two disconnected components $A$ and $B$, as described above. (We will now attach $A$, $B$, or $C$ as subscripts to a variety of quantities, to indicate that they are associated with one of these clusters). Consider the structure of $H_C^{\text{eff}}$ for the single-flipped-spin states. At order $\lambda^0$, the states on which $H_C^{\text{eff}}$ acts have a flipped spin in one of either $A$ or $B$ and no flipped spin in the other component, and it should be clear that even as $\lambda$ is increased from zero, and the states develop more structure, that there is no way for the spin-flip to “jump” between disconnected parts of the cluster. In other words, we assert that if we start with an unperturbed state in which there is a spin-flip in subcluster $A$ but no spin-flip in $B$, and apply $H_1$ (more precisely, the restriction of $H_1$ to $C$) any number of times, the resulting state will have zero overlap with any unperturbed state in which there is a spin-flip in $B$ but none in $A$. What this implies is that $H_C^{\text{eff}}$ has a block-diagonal form, specifically,

$$H_C^{\text{eff}} = [H^{\text{eff}} + e_B I]_A \oplus [H^{\text{eff}} + e_A I]_B$$

(10)

where $e_A$ denotes the ground state energy of cluster $A$ and $I$ is the identity operator. Thus
$H^{\text{eff}}$ itself does not have a cluster expansion, since it is not simply additive for a disconnected cluster. However, if we subtract $e_C = e_A + e_B$ from all the diagonal elements on both sides of the equation above,

$$[H^{\text{eff}} - e_CI]_C = [H^{\text{eff}} - e_AI]_A \oplus [H^{\text{eff}} - e_BI]_B,$$

we see that $H^{\text{eff}} - eI$ does have a cluster expansion. In carrying out subgraph subtraction, one must keep track of which sites in the graph correspond to which sites in the subgraph, and the subtract all of the appropriate matrix elements, order by order. As a check of the validity of the calculation, one should find that the weight for $H^{\text{eff}} - eI$ on a cluster with $p$ terms of $H_1$ should vanish identically up to order $\lambda^{p-1}$.

Once the weights have been evaluated for all graphs contributing up to a desired order in $\lambda$, the excited state dispersion is trivial to evaluate. Each matrix element in the weight of $H^{\text{eff}} - eI$ for each cluster is associated with some vector on the lattice. One must simply sum all of the matrix elements associated with any given lattice vector $r_s$; denote the resulting sum of (power series of) matrix elements by $t_s$. The effective Hamiltonian in the single-flipped-spin sector for the infinite lattice is now known to the desired order in $\lambda$, and it is diagonalized by plane-wave eigenfunctions. The resulting dispersion relation for the excitation energy associated with a spin-flip is $\sum_s t_s \exp(iq \cdot r_s)$.

Just as in the case of ground-state expansions, one should take advantage of geometric and topological classification of the clusters in order to avoid redundant calculations: but that is a well-understood technical detail that requires no further discussion here.

We have in fact implemented the algorithm described above for the $S = 1/2$ transverse-field Ising chain, and reproduced the exactly-known dispersion $[1 + 2\lambda \cos q + \lambda^2]^{1/2}$ to order $\lambda^{11}$ (and for this model it would be easy to push the calculations further). Upon being informed of the algorithm, Singh [7] promptly carried out the analogous calculation for the single-flipped-spin excitations of the $S = 1/2$ square-lattice Heisenberg-Ising antiferromagnet; by appropriate extrapolation to the Heisenberg limit he directly obtains a value of the spin-wave velocity which is consistent with the current best estimates.
Similar calculations of elementary excitation spectra for other models would be straightforward; however, they do not exhaust the potential applications of this method. The “eigenvectors” $|\psi^{(l)}\rangle$ contain information on correlations in the vicinity of the excitation. The set of overlaps (in the context of the transverse-field Ising model, for concreteness) $\langle \psi | \sigma^x_l | \psi^{(l)} \rangle$, where $|\psi\rangle$ is the perturbatively-constructed ground state of the cluster, should contain all the information needed to evaluate the quasiparticle residues associated with the elementary excitations. In fact a calculation of the residues has already been accomplished for the Heisenberg-Ising antiferromagnet, and will be reported separately. One subtle point worth emphasizing here is that the method of constructing $H_{\text{eff}}$ is a similarity transformation but not a unitary transformation. Insofar as the calculation of the spectrum is concerned, the distinction is irrelevant. However, the states $|\psi^{(l)}\rangle$ are not orthogonal, and this fact must be carefully taken into account whenever they are used in further calculations.

Another interesting extension would be to “two-particle” excited states. Here the situation is rather more complicated than for “single-particle” excitations such as the one-flipped-spin states of the transverse field Ising model, on two counts. First, the two-particle effective Hamiltonian for the infinite lattice is not, in general, trivially diagonalizable like in the one-particle case. So the value of this method would be to yield a finite number of terms in an exact series expansion for the quasiparticle interactions: the next step would be along the lines of traditional many-body theory, or perhaps even exact diagonalization! (One would have dramatically reduced the size of the Hilbert space, compared to exactly diagonalization of the original model, but at the cost of introducing more complicated, long-range interactions.) Second, the analog of Eq. (11) is considerably more difficult to write down, and it is not clear precisely what quantity exhibits a cluster expansion. We believe these issues merit examination in future work, as well.

At this point it is possible to sensibly compare the method outlined here with the few other series expansions methods for excited states which exist in the literature. Expansions for the elementary excitation spectra of the transverse-field Ising model on various lattices, and of the dimerized Heisenberg antiferromagnetic chain, were carried out some years ago.
by Pfeuty and Elliott \cite{8} and Harris \cite{9}, respectively. Neither of these methods is in the form of an explicit cluster expansion, nor do they appear to be readily implementable as a computer program, as required for high-order calculations. So far as we are aware these methods have not seen further use.

Barber and Duxbury \cite{10} constructed the expansion for the lowest excitation energy in the next-neighbor transverse field Ising chain via Rayleigh-Schrödinger perturbation theory on finite rings. Because this is not a cluster expansion method it cannot be efficiently extended to higher-dimensional lattices, and it is not clear whether it can be adapted so as to yield the entire elementary excitation spectrum, either. However, this approach has been applied to other one-dimensional models (see for example \cite{11}).

Finally, there is a method which is due to B. G. Nickel \cite{12} and which has been applied by Hamer and coworkers to several spin models \cite{3,13}. This method is almost a cluster expansion; to be precise a finite set of disconnected clusters need to be included as well as the connected clusters. It is also limited to the lowest excitation energy only.

What sets the method presented in this paper apart from those already reported in the literature is the recognition that there is an excited state quantity which is additive over disconnected clusters, so that the usual machinery of connected-cluster expansions can be applied. Because this quantity turns out to be the effective Hamiltonian in the single-particle excitation subspace, one can obtain the entire elementary excitation spectrum as readily as the gap.

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