Augmented space formalism and renormalization for ground and excited states of magnetic systems

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Abstract. The augmented space formalism has been used so far for the study of disordered crystals. We stress here that the topological structure of the augmented space of a binary alloy is formally equivalent to the set of configurations of an Ising system. In particular in both cases a very useful binary representation for labelling the vectors of the space can be done. Starting from this observation we have developed a very efficient description of the Ising Hamiltonian, and we have shown that it can be successfully applied both in the direct diagonalization approach and in conjunction with the renormalization scheme. Within this last case we have proposed a generalization of the techniques commonly used in the literature, obtaining very good results.

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I. Introduction

In this paper we present an application of the augmented space formalism [1–7] (up to now used in the literature for the study of the properties of alloys) to magnetic systems. Our work lies on the observation that the set of configurations of an Ising system is formally equivalent to the augmented space for a binary alloy with the same number of sites: this allows to extend the methods developed in the framework of the disorder theory to magnetic spin systems. In particular we find useful a binary representation [8] for labelling the states when direct diagonalization of the Ising Hamiltonian [9] is done either by standard linear algebra [10] techniques of by Lanczos [11–14] and modified Lanczos [15] procedures. The renormalization approach has also been used [16–19], to handle Ising Hamiltonians. We propose here an improved renormalization procedure which allows to represent the original infinite system in terms of the eigenvalues and eigenvectors of finite clusters which are iteratively renormalized up to convergence. We obtain thus a careful determination of the critical field and of the thermodynamic properties of the magnetic system.

We use real space renormalization group in the spirit followed by Jullien et al. for the study of the Kondo impurity problem [20] and of the quantum Ising model [21]. It consists in the solution of the infinite system into blocks of spins whose low energy states only are retained, so that after suitable inflation of the blocks the ground and the very few low lying excited states of the overall systems are obtained. We propose here a generalization of this method to obtain any desired excited state of the system, in terms of a recently presented modified Lanczos algorithm [15]. The exemplification of our procedure to the case of the Ising model in a transverse field is mandatory; it is in fact a prototype one dimensional model of great interest due to its analogy with other phase transition problems [22].

In Sect. II we first describe the Hamiltonian of each cluster by means of the binary logic technique; in Sect. III we present an efficient procedure for the calculation of eigenvalues and eigenvectors based on a recent modified version of the Lanczos procedure. Section IV is devoted to the application of our scheme to the standard renormalization procedure. In Sect. V we propose a generalization of the above renormalization procedure. Section VI contains the conclusions.

II. Augmented spaces and clusters spins

Let us consider the following Hamiltonian for the one-dimensional Ising spin system in a transverse field [9]:

\[ H = \sum_{i=1}^{N} \left( -h \sigma_{x}(i) - J \sigma_{z}(i) \sigma_{z}(i+1) \right) \] (1)

where \( \sigma_{x}(i) \) takes the values +1 or −1 if the site \( i \) is occupied by a spin up or by a spin down respectively and \( \sigma_{x}(i) \) causes the spin flip at the site \( i \); \( J \) is the nearest neighbour interaction and \( h \) is the external magnetic field.

The matrix elements of the Hamiltonian (1) can be easily described by the binary logic representation for
ground and excited states already successfully employed in
the augemented space formalism for substitutional binary
alloys [8]. For this aim let us first decompose the system
in terms of identical clusters with N sites. As a basis for the
hamiltonian (1) we choose the $2^N$ configurations accessible
to each cluster. These configurations are build up in the
following manner: the first configuration has all the spins
down (ground state); then we have N configurations with
one spin up and $N - 1$ spin down, then there are $N(N - 1)/2$ configurations with two spins up and $N - 2$
spins down, and so on. The evaluation of the matrix
elements of the hamiltonian (1) on this basis can be done
along the following points.

1) Given an integer $n$ between 0 and $2^N - 1$ we con-
struct the N-dimensional vector $\eta$ whose j-th component
is the value of the bit j in the binary representation of the
integer n; this vector can be associated to a configuration.
In fact it is worthwhile to notice that if we assume the
convention that a spin up corresponds to a bit one and
a spin down to a bit zero each configuration is the binary
representation of an integer between zero and $2^N - 1$. It is
evident that the binary representation allows to store
a configuration without the knowledge of the actual
values of the spin in each site but only assigning the
integer that unambiguously labels the configuration itself.
The procedure to obtain the binary representation of an
integer is well known from aritmetics, and, for a given
value of $n$, can be summarized in the following flow-chart:

\begin{align}
\eta(j) &= \text{mod}(n, 2) \\
n &= n/2 \\
\text{repeat}
\end{align}

where the function mod is the rest in the division of
integers.

2) The diagonal (same configuration) matrix elements
of the hamiltonian are simply a sum of + 1 and - 1
factors (times $-h/2$) depending upon the value (1 or 0) of
the bits in the binary representation of the integer corre-
sponding to the configuration:

$$H_{n,n} = - \sum_{j=1}^{N} (\eta(j) - \frac{1}{2})h$$

3) As far as the off-diagonal interaction is concerned,
we notice that it is present only between configurations
differing for the values of two adjacent spins; thus, from
the binary representation of any binary configuration we
calculate the $2^N - 1$ configurations differing from it for the
value of two adjacent spins: in this way we know all the
nonzero off-diagonal connections (all equal to $J$) in the
hamiltonian. Operatively the procedure can be carried on
by defining an auxiliary vector $\eta'(j)$:

$$\eta'(j) = \eta(j) \quad j \neq k, k + 1$$
$$\eta'(k) = 1 - \eta(k)$$
$$\eta'(k + 1) = 1 - \eta(k + 1)$$
$$k = 1 \ldots N - 1.$$  

Then the integer corresponding to $\eta'(j)$ can be calculated
passing from binary to decimal basis:

$$m = \sum_{j=0}^{N-1} \eta'(j) 2^j.$$

Finally we can write the (nearest-neighbour) off-diagonal
matrix element:

$$H_{m,n} = - J.$$  

For chosen dimension of the one dimensional cluster, the
hamiltonian (1) can be diagonalized using standard rou-
tines [10] or the recursion method [11-14]. Operating
with this last technique it is convenient to use the modified
Lanczos procedure [15] that allows a precise determina-
tion of all excited eigenvalues without the need to calcu-
late the complete spectrum of the hamiltonian; this is just
the case which we are interested in, when calculating the
mass gap (see later) or when looking for the free energy
limited to the lowest eigenvalues. Let us see now in detail
how the calculation of eigenvalues is performed.

III. Cluster diagonalization by modified Lanczos procedure

Before passing to the description of the modified Lanczos
method, a brief resume of the standard recursion procedure
is worth. Let us consider an arbitrary operator $H$, whose
representation on a given orthonormal basis set $\{|0\rangle\}$ is known. Starting from an initial state $|u_0\rangle$ given
by a linear combination of the basis states $\{|\phi_i\rangle\}$, a hier-
archical chain of orthonormalized states $|u_0\rangle, |u_1\rangle, |u_2\rangle...$
... is constructed using the three-terms recurrence relation:

$$|U_{n+1}\rangle = (H - a_n)|u_n\rangle - b_{n+1}|u_{n-1}\rangle;$$

the coefficients $b_{n+1}$ and $a_{n+1}$ at the $n + 1$-th iteration step
are given by the relations:

$$b_{n+1} = \langle U_{n+1} | U_{n+1} \rangle \tag{6.a}$$
$$a_{n+1} = \frac{H \langle U_{n+1} | U_{n+1} \rangle}{\langle U_{n+1} | U_{n+1} \rangle} \tag{6.b}$$

The practical usefulness of the new basis $\{|u_n\rangle\}$ is that the
hamiltonian is tridiagonal on it; moreover the diagonal
matrix element of the resolvent on the state $|u_0\rangle$ has the
following continued fraction expansion [13, 14]:

$$G_{00}(E) \equiv \langle u_0 | \frac{1}{E - H} | u_0 \rangle = \frac{1}{E - a_0 - \frac{b_1^2}{E - a_1 - \frac{b_2^2}{E - a_2 - \cdots}}} \tag{7}$$

Let us now consider how this procedure may be used to
obtain a variational derivation of the ground state eigen-
value of $H$. For this aim, the iterative procedure of eqs. (5)
and (6) are performed only once, obtaining a couple of
orthonormal states $|u_0\rangle$ and $|u_1\rangle$. Then the operator $H$ is
diagonalized within the subspace spanned by $|u_0\rangle$ and
$|u_1\rangle$ (Krylov subspace) and the eigenvector corresponding
to the lowest eigenvalue is taken as initial state for the next