Ising-like models on arbitrary graphs: the Hadamard way

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We propose a generic framework to analyse classical Ising-like models defined on arbitrary graphs. The energy spectrum is shown to be the Hadamard transform of a suitably defined vector associated with the graph. This allows a quick computation of this spectrum owing to the existence of a fast Hadamard transform algorithm (used for instance in image compression processes). We then go further and apply this formalism to regular graphs, such as hypercubic graphs, for which a simple recurrence relation for the spectrum is given, which speeds up even more its determination. First attempts to analyse partition functions and transfer matrices are also discussed.

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I. INTRODUCTION

Ising-like interactions enter paradigmatic sets of models defined to describe phase transitions in statistical physics, and has been applied to a very large set of a priori different problems, even outside physics. It is clearly not achievable to summarize in few words the many contributions on that subject, and the interested reader is sent to the numerous review papers or books, see for instance ref. Nevertheless useful to recall is the initial Ising-Lenz solution for the 1-dimensional case, and the absence in that case of phase transition at positive temperature, the Peierls proof for the existence of a phase transitions in 2 dimensions, followed later on by the Onsager solution. Up to now, and even though a large amount of work gives precise informations about the phase diagram in three dimensions, no exact solution is known in that case.

In this paper, we intend to present a generic framework for such cases where classical two-level spins located at graph vertices interact through n-body terms, the well known Ising model corresponding to one- and two-body interactions. We show how some simple algebraic tools can be used to describe and speed up the numerical solution of the spectral problem defined on an arbitrary graph. Although this formalism apply to generic models with n-body interactions, which can be either regular or disordered, we shall mainly concentrate our presentation on the standard Ising model. In a first step, we define a binary vector which fully describe the graph structure, and a “coding vector” which embodies the Hamiltonian. We then show that, under an Hadamard transformation, this coding vector is sent to a “spectral vector”, whose components are the set full set of energies in the configuration space. An important point here is to recall the existence of a “Fast Hadamard Transform” (FHT), able in principle to considerably speed up the computation.

We then concentrate on some regular graphs (mainly hypercubes), for which even stronger results can be derived. Finally, some preliminary attempts to adapt this formalism to transfer matrix and partition function determination will also be presented.

II. ISING-LIKE MODELS ON ARBITRARY GRAPHS

A. Ising-like hamiltonian

We consider a graph $G$, with its $N$ vertices gathered in a set $V$ and its bonds, as pairs of neighbouring vertices, in a set $B$. The simplest Ising model describes classical spins $S_i = \pm 1$ located at the $G$ vertices, subject to a constant magnetic field $h$, and to constant pairwise interactions for spins connected by a graph edge. The spin configuration space is the product $(\pm 1)^{\otimes N}$, forming a hypercube $\Gamma_N$ in $N$ dimensions, with its $M = 2^N$ vertices encoding the possible spin states in $G$. The Ising model associates to each vertex in $\Gamma_N$ an energy:

$$E_{\{S_i\}} = J \sum_{<i,j> \in B} S_i S_j + h \sum_{i \in V} S_i, \quad (1)$$

with $J < 0$ (resp. $> 0$) favouring ferromagnetic (resp. antiferromagnetic) ordering. For sake of presentation, we shall mainly discuss here the Ising model regular case, with equal $h$ and $J$ terms for all sites and bonds. However, most of what will be said below in the first part, with respect to the Hadamard Transform action, apply as well to disordered (spin glass) problems, and even to n-body interactions.
B. Coding graphs and interacting hamiltonians into binary vectors

In general, a graph is rather faithfully described by its adjacency $N \times N$ matrix $A$, with $A_{ij} = 1$ whenever sites $(i, j) \in B$ and zero instead. But, especially for non-planar graphs, we may be interested in having a finer description, pointing onto higher dimensional cells of the graph (faces, polyhedra, polytopes ...). A simple generic binary vector $|G\rangle$ of size $2^N$, in a space with basis $B = \{0, 1\}^\otimes N$ fulfill this task in the following way: a basis vector is an ordered sequence of 0 and 1. Each binary digit position will correspond to a vertex of the graph; the occurrence of these different vertices in the graph is marked by a component 1 for the basis vectors having one 1 at the site position and $N-1$ zeroes elsewhere. A n-cell of the graph is a subset of $n$ vertices; its presence in the graph is encoded in $|G\rangle$ as a component 1 for the basis vector having $n$ terms equal to 1 at these vertices position and zero elsewhere.

The next step is to code the interacting n-body spin Hamiltonian as a coding vector $|C\rangle$. The interacting terms are associated to n-body cells: the external magnetic field act onto one-body cells (vertices), the standard Ising interaction onto (two-body) edges, etc ... The vector $|C\rangle$ has non vanishing components, equal to the related n-body interaction term, precisely for those basis vector which code the corresponding n-body cell in $|G\rangle$. As a very simple example, a graph composed of 2 vertices joined by a bond will be characterized, in the basis ${|00\rangle, |01\rangle, |10\rangle, |11\rangle}$, by $| G >= (0, 1, 1, 1)$, and its (Ising model) coding vector as $| C >= (0, h_1, h_2, J_{1,2})$; the site position is ordered here from right to left, as in standard binary decomposition. Notice also that we are now switching from the above $(\pm 1)^\otimes N$ spin configuration notation to the equivalent $\{0, 1\}^\otimes N$ one with, say, implicit bijection between +1 (or $\uparrow$) to the binary label 0.

III. ISING SPECTRUM FROM HADAMARD TRANSFORM

A. Hadamard Transform

We describe now how to simply compute these interacting spin models spectra, eventually leading to a natural speed up in their numerical derivation. The spectrum has $M$ terms (therefore exponential with $N$), discretely ranging in an interval which generically grows linearly with $N$. It is therefore, as is well known, highly degenerate, in a way which cannot be solely captured by the graph $G$ and global spin symmetries. We propose here to analyse this spectrum with tools analogous to the Fourier transformation, but adapted to the peculiar $\Gamma_N$ hypercube geometry. This is precisely the task fulfilled by the so-called Hadamard Transform H.T. (one sometimes finds additional names associated to it, like Walsh and Rademacher), which is a linear transformation on a $2^N$-dimensional space, given, with the standard basis $\{0, 1\}^\otimes N$, by the $2^N \times 2^N$ Hadamard matrix $H_M$ defined recursively (with $H_0 = 1$) as

$$H_{m+1} = \begin{pmatrix} H_m & H_m \\ H_m & -H_m \end{pmatrix}; \text{ with } H_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \text{ and } H_2 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

(2)

A normalization factor $1/\sqrt{2}$ is often multiplied on the RHS for $H_1$, but will only prove useful in the second part of this presentation. The above relation reads also $H_{m+1} = H_1 \otimes H_m$; one easily also gets that $H_{p+q} = H_p \otimes H_q$. Hadamard matrices have the nice property that their rows or columns are pairwise orthogonal. The component $H_{p,q}$, with line $p$ and row $q$ both starting from zero, can be written in a compact way, by considering the base 2 decomposition $p_j$ and $q_j$ of $p$ and $q$:

$$H_{p,q} = (-1)^{\sum p_j q_j}$$

(3)

B. The Hadamard transformed coding state

For a given spin configuration, each bond contributes through a term $\pm J$ to the energy, according to whether the two spins points to similar or opposite directions. In addition, each site contributes by $\pm h$ according to the local spin orientation. The complexity in computing the spectrum amounts to adding “coherently” these contributions for each $\{S_i\}$ configuration. Coherent addition of amplitudes is precisely what the quantum framework knows how to deal with. This is why, although not a necessity, we shall adopt quantum-like notations to describe our proposed recipe.

Let us write the Ising hamiltonian for quantum spins (in the $S^z$ basis) with Pauli matrices instead of classical spins (only $\sigma^z$ matrices are used, so no added quantum complications)
\[
\mathcal{H} = J \sum_{<i,j> \in B} \sigma^x_i \sigma^x_j + h \sum_{i \in V} \sigma^z_i \quad (4)
\]

Let \(|0\rangle\) be the fully polarized (which could be called here a vacuum state) in the initial standard \(\sigma^z\) basis. As easily checked, the above Ising coding state simply reads \(|C\rangle = \mathcal{H} |0\rangle\).

We now define the spectral state \(|E\rangle\) as the Hadamard Transform of \(|C\rangle\): \(|E\rangle = H_N |C\rangle\). The main first result of this paper states that \(|E\rangle\) have components which are precisely the energies of the associated classical Ising model we started with, a point which can be understood by considering carefully how the above \(H_{p,q}\) terms enters the matrix action in the Hadamard transformation. Notice that, interestingly, in the quantum spin context, this amounts to a basis change from the \(\sigma^z\) to the \(\sigma^z\) basis (a basis change precisely done by \(H_N\), if the above mentioned normalization factor \(1/\sqrt{2}\) is introduced). \(|C\rangle\) is the superposition of an entangled bond vector \(B := J \sum_{<i,j> \in B} \sigma^x_i \sigma^x_j |0\rangle\) and site vector \(S := h \sum_{i \in V} \sigma^z_i |0\rangle\). The Hadamard Transform of a given component, say \(\sigma^x_i \sigma^x_j |0\rangle\), peaks out a factor \(\pm 1\) according to whether spins\((i,j)\) are parallel or not (see expression (3)). The contributions are then added coherently, and the total amplitude is precisely the corresponding Ising classical energy.

Notice that the Hadamard Transform has already been mentioned in the context of spin glass Ising models\(^5\), but used quite differently. Here, the introduction of the spectral vector \(|E\rangle\) as the Hadamard transform of the coding state makes its role direct and transparent.

To illustrate our approach, let us describe the simplest cases of two and three spins forming a bond and a triangle. With \(N = 2\), the coding state has already been given above, and the spectral state reads

\[|E\rangle_{2} = (2h + J, -J, -J, -2h + J)\]

whose components are indeed the classical Ising energies. With \(N = 3\), the coding state reads \(|C\rangle = (0, h, h, J, h, J, J, 0)\), which is transformed by \(H_3\) to the Ising amplitudes

\[|E\rangle_{3} = (3h + J, h - J, h - J, -h - J, h - J, -h - J, -h - J, -3h + J)\]

C. Discussion

We end this first part by a set of remarks:

1. Fast Hadamard Transform.

Up to now, the above presentation may sounds just as a reformulation, even though nice in itself, of the Ising model. However a quite interesting feature arises from the existence of a Fast Hadamard Transform algorithm, widely used for instance in early digital image compression\(^{6}\), which therefore should provide a very fast way to compute the Ising spectrum for an arbitrary graph once the coding state is known. FHT relies upon the above iterative construction of \(H_{m+1}\) from \(H_1\) and \(H_m\), which iteratively “block diagonalize” the transformation. As a result, the Hadamard Transform, which would present in standard implementation a computational cost of \(O(m^2)\), with \(m\) the linear matrix size, is now turned into an algorithm of \(m \log m\) complexity. Whether the use of FHT would significantly speed up spectral computations is certainly worth to be further checked. In particular, our proposed framework is memory consuming (the coding state has size \(2^N\)), but, although not evident for the above two examples with 2 and 3 spins, this coding state is generically a sparse vector.

A simple way, alternative to the FHT, to deal with the sparseness of \(|C\rangle\) would be to focus on those Hadamard matrix columns corresponding to the non vanishing elements of the coding states; such a column is readily computed as a tensor product of \((1, 1)\) and \((1, -1)\) column vectors, corresponding to the ordered occurrences of “0” or “1” in the binary decomposition of the column position ( where, as for the derivation of expression\(^5\) the first column start at position 0). This already produces a very fast way to compute the spectrum.

2. Extension to more complex models.

Up to now, we have concentrated on the regular Ising model model, with constant \(J\) and \(h\) parameters. However, inspection of expression\(^5\) shows that the coherent addition of interaction contributions pertains for non regular
parameters. A spin glass-like coding state, where disorder affects either the local magnetic field or the couplings (or both) will also lead to the correct spectral state. Even more, as again can be checked from expression 3, generalized classical spin 1/2 models containing n-body interactions can be treated equally.

3. Experimental implementation.

As noted above, the Hadamard Transform operates a basis change from the the $\sigma^z$ to the $\sigma^x$ basis. This opens the possibility for an interesting experimental implementation: first prepare the (generically) entangled coding state in the $\sigma^z$ basis, and then measures this state in the $x$ orientation. Recall however that the spectral state $|E>$ has the Ising energies as “probability” amplitudes, which should be squared to compare with experimental occurrences (and therefore would not distinguish two energies opposite in sign). We do not claim here that this would give for sure an operational method to compute large size Ising models spectra. But, with an entangled coding state to be prepared, and quantum coherence to be achieved through the Hadamard Transform, it could already provide an interesting test for any quantum machine claiming to work in a quantum regime.

4. Transformation paths from the coding to the spectral state.

The standard Fourier transform relates a real and a dual reciprocal (or momentum) space. We see here that the Hadamard transform (which can be viewed as a multidimensional discrete Fourier transform) relates a vector coding interactions on a graph to a (dual) vector coding the corresponding Ising energies. Suitably normalized, the Hadamard transform is a unitary transformation; it was then rather tempting to follow continuously this transformation in spin space, ending at the full Hadamard Transform, and see what could be learned from this. Some preliminary attempts on small systems display interesting but complex patterns for the amplitudes and the degeneracies, but did not allow us to reach a clear understanding of the coding state trajectory.

A different approach would consist in applying the H.T. spin after spin, following a discrete path to reach the full Hadamard Transform. In fact, a close inspection shows that it is precisely how the Fast Hadamard Transform algorithm works.

IV. ISING MODEL ON REGULAR STRUCTURES

By a regular structure we mean here a structure which can be built iteratively by adding identical substructures. A simple case is provided by an hypercube $\gamma_d$ in dimension $d$, made of two $\gamma_{d-1}$ (note that, hypercubes being ubiquitous here, we use “$\gamma$” for the structure, and “$\Gamma$” for the configuration space). We show now that, for such regular structures, the spectral state $|E>$ can be computed iteratively in a rather efficient way, even compared to a direct use of standard FHT. The demonstration will use some algebraic tools that are first recalled. Notice that the proposed framework also apply, as a one-step procedure, for line to line or plane to plane addition in a lattice and allows therefore for standard transfer matrix constructions, which are discussed in a second step.

A. Some definitions and notations

Let us first recall some linear algebra operations, and define related notations, that will prove useful below. All are elementary, but at the same time refer to sometimes unusual tools (at least for a physicist) like matrix Hadamard product or vec-like operators.

We write $I_n$ the identity matrix of size $n$, $1_n$ the $n \times n$ matrix made of 1, and $|1_n>$ the corresponding size $n$ vector. For a vector $|X>$, we define the diagonal matrix $D_{|X>}$ whose componant $D_{jj}$ is the $j^{th}$ componant $X_j$.

1. Hadamard products

The matrix Hadamard product “$\circ$”, also called entrywise product, multiplies pairwise elements of two matrices to form a third one ($C = A \circ B$, such that $C_{ij} = A_{ij}B_{ij}$). We shall also use below a “vector Hadamard product” $|A > \circ |B>$ whose componants are the pair-wise product of componants, and a left (resp. right) Hadamard product
of a vector and a matrix, which amounts to multiply the matrix $i^{th}$ row (resp. column) by the $i^{th}$ component of the vector. Notice that, for a matrix $M$ and vector $|A\rangle$ of same linear size,

$$|A\rangle \circ M = D_{|A\rangle} M, \text{ and } M \circ |A\rangle = M.D_{|A\rangle}$$

Having in mind the usual function elementary expansion, we shall call $\circ \exp$ the “Hadamard matrix exponential” whose effect is $(\circ \exp A)_{ij} = \exp(A_{ij})$, and extend this definition to vectors. We shall eventually use the (trivial) relation:

$$\circ \exp (|A\rangle + |B\rangle) = \circ \exp(|A\rangle) \circ \exp(|B\rangle)$$

2. A “special” sum for matrices and vectors

We define special matrix and vector sums $\uplus$ as:

$$\begin{cases}
A \uplus B = A \oplus 1_n + 1_n \otimes B \\
|A \uplus |B\rangle = |A \rangle \otimes |1 \rangle + |1 \rangle \otimes |B\rangle,
\end{cases}$$

where the subscript $n$ (the vector size) has been omitted, and $\otimes$ is the standard Kronecker product. Be careful not to confuse with the standard matrix Kronecker sum $A \oplus B = A \otimes I_n + I_n \otimes B$ where the identity matrix $I_n$ appears instead the “one matrix” 1. Notice the useful relation:

$$\circ \exp (A \uplus B) = \circ \exp A \otimes \circ \exp B,$$

which reminds (but differs from) the better known $\exp(A \oplus B) = \exp A \otimes \exp B$ involving the standard matrix exponential and Kronecker matrix sum.

3. The vec operator

The vec operator maps a $n \times m$ matrix onto a column vector of size $n \times m$, simply built by stacking the successive columns of the original matrix. We are mainly interested here by square matrices, and would like also to use the inverse of a vec map, unravelling a vector of size $n^2$ onto an $n \times n$ matrix with its successive columns taken from the vector components. There is an apparent notation conflict here, some authors calling devec this operator, while others use vec to denote the operator building a row vector of size $n \times m$ from the original matrix by concatenation of its successive rows. Therefore we shall adopt here the notation unvec for the inverse of vec. The following useful identity, involving three matrices $P, Q$ and $R$ will be used later:

$$\text{vec}(P,Q,R) = (R^T \otimes P).\text{vec}(Q),$$

where $R^T$ is the matrix transpose of $R$, and the “dot” refers to the standard product for matrix algebra (between two matrices or a matrix and a vector).

B. The hypercube case

We now discuss a recursive algorithm to compute the Ising model spectra for the family of hypercubes with increasing dimensionality. Notice that, interestingly, a hypercube $\gamma_{2d}$ is topologically equivalent to an hypercubic lattice of lateral size 4 in dimension $d$, with periodic boundary conditions (PBC), noted here $Z_4^d$. The latter inherits the former symmetry group, of order $(2d)!2^{2d}$. The hypercube $\gamma_d$ has $N = 2^d$ sites; its spin configuration space is the hypercube $\Gamma_M$ with $M = 2^N$. The recursive additive construction $\gamma_{d+1} = \gamma_d \cup T(\gamma_d)$, where $T(\gamma_d)$ is a translated version of $\gamma_d$ in the new space dimension, leads to a Kronecker product for the respective configuration space: $\Gamma_{M^2} = \Gamma_M \otimes \Gamma_M$. 

1. Ising addition spectrum for two uncorrelated subgraphs

Let us start by trivially writing the spectral vector for the union of two graphs $G_1$ and $G_2$, both with $N$ sites for sake of simplicity, but with possibly different interaction coding states (Ising model parameters). Compute first (say through FHT) the two spectral states $|E_1\rangle >$ and $|E_2\rangle >$. If the two graphs have no interactions, the spectral state of their union $G$, noted $|E\rangle >$, is simply the “addition spectrum” of its two parts, an object which is precisely given by the above defined special vector sum $\oplus : |E\rangle > = |E_1\rangle > \oplus |E_2\rangle >$.

The latter expression can be easily checked directly; let us nevertheless derive it in the present framework. Call $|0\rangle_N$ the fully polarized state with $N$ spins, and $|C_1\rangle$ and $|C_2\rangle$ the coding states associated to $G_1$ and $G_2$. Since up to now the latter are not Ising connected, the coding state for $G$ simply reads

$$|C\rangle = |C_2\rangle \otimes |0\rangle_N + |0\rangle_N \otimes |C_1\rangle.$$  \hfill (12)

$|0\rangle_N$ is the first element in the standard basis $\{0,1\}^\otimes N$, and its Hadamard Transform is easily shown to be $|1\rangle_N$. As a result, the spectral state $|E\rangle$ reads

$$|E\rangle = H_{2N} \cdot |C\rangle = (H_N \otimes H_N) \cdot |C\rangle = |E_2\rangle \otimes |1\rangle_N + |1\rangle_N \otimes |E_1\rangle > = |E_2\rangle > \oplus |E_1\rangle >$$  \hfill (13)

Now real interesting questions start when the graphs union is dressed with new couplings between the parts, with the task of combining coherently these new interactions with the simple “disconnected” addition spectrum.

2. Introducing interactions between the subgraphs

There are clearly three types of Ising (bond) interactions: those associated separately to $G_1$ or $G_2$, and those connecting the two graphs. For reasons which will be clear below, we choose to consider the matrix $C_{2N} = \text{unvec}(|C_{2N}\rangle)$). The first two types of bonds appear in its first column as the column vector $|C_1\rangle >$, and in its first row as the line vector $< C_2 |$, a direct consequence of the above uncorrelated graph coding state in formula (12). The remaining part, forming a matrix $D$, codes the remaining interactions. It has non vanishing elements only at positions corresponding to an interacting bond between the graphs $G_1$ and $G_2$. At this stage, this description is still generic and applies to the union of two different graphs, with possibly non regular bonding between the two graphs, the complexity being coded in $D$. We now show that for the class of regular graphs to which hypercubes belong, $D$ takes a simple form which allow for a recursive analysis.

3. Ising spectrum for the hypercube

The additive construction of hypercubes translates into a simple iterative construction for the coding state vector from $|C_N\rangle >$ to $|C_{2N}\rangle >$. If we are cautious enough to number the sites coherently for the two $\gamma_d$ copies (which means sites $j$ and $j+N$ are translation related), we get a rather simple form for the matrix $D$ which turns into a pure diagonal matrix, the third type of bonds contributions sitting at location $2^J + 1$ along the diagonal, with integer $j$ running from 0 to $N-1$, and being simply related to the above defined site vector $|S_N\rangle >$ associated to $\gamma_d : D_{2N} = J D_{|S_N\rangle}$.

To clarify our notations, let us display these objects for the easiest case, from the point $\gamma_0$ to the segment $\gamma_1$ and then to the square $\gamma_2$ :

$$|C_1\rangle > = \begin{pmatrix} 0 \\ h \end{pmatrix}, \quad |C_2\rangle > = \begin{pmatrix} h \\ J \end{pmatrix}, \quad C_2 = \begin{pmatrix} 0 & h \\ h & J \end{pmatrix}, \quad D_2 = \begin{pmatrix} 0 & 0 & h & J \\ h & 0 & 0 & J \\ J & 0 & 0 & 0 \end{pmatrix}, \quad D_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & J & 0 & 0 \\ 0 & 0 & J & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$  \hfill (14)

We aim to compute the Ising spectrum vector $|E_{2N}\rangle = H_{2N} \cdot |C_{2N}\rangle >$. This could be done easily using FHT as discussed above. But we proceed differently here, by recalling that $H_{2N} = H_N \otimes H_N$ and that $H_N^T = H_N$. We then use relation (11), with $P = R = H_N$ and the above defined $C_{2N}$ to get:

$$|E_{2N}\rangle > = \text{vec} (H_N.C_{2N}.H_N)$$  \hfill (15)

This only difficult part requires now to evaluate a set of matrices $M_{2N} = H_N.D_{2N}.H_N$, the Hadamard transformed $D_{2N}$ matrices, which happens to follow a simple iterative construction. Some easy algebra leads to the following coupled system, which iteratively constructs the hypercube Ising spectrum in any dimension :
\[ \left\{ \begin{array}{l}
E_{2N} > = (E_N > \psi | E_N >) + \text{vec}(M_{2N}) \\
M_{2N} = M_N \psi M_N
\end{array} \right. \] (16)

As already said, the first term on the RHS of the first equation provides the expected addition spectrum from the two copies of \( \gamma_n \), while the second term contains their interaction. We let as an exercise to the interested reader to recover, from the initial \( | E_1 > = (h,-h) \) and \( M_2 = \text{unvec}(J,-J,-J,J) \), the Ising spectrum for a square:

\[ | E_4 > = (4h + 4J, 2h, 2h, 0, 2h, 0, -4J, -2h, 2h, -4J, 0, -2h, 0, -2h, -2h, -4h + 4J) \] (17)

Relation (16) is very easily iterated numerically. As an example, two additional iterations leads, almost instantaneousy on a standard computer, to \( | E_{16} > \), the spectrum for \( \gamma_4 \), and therefore for the \( 4 \times 4 \) square lattice system with periodic boundary conditions. It reads, with \( J = 1 \) and \( h = 0 \), given in frequency (pairs of numbers, first term for the energy, and second term its degeneracy):

\[ \{-32, 2\}, \{-24, 32\}, \{-20, 64\}, \{-16, 424\}, \{-12, 1728\}, \{-8, 6688\}, \{-4, 13568\}, \{(0, 20524)\}, \ldots \] (18)

We omit the positive part of the spectrum, the latter being symmetrical. Notice however that iterating relation (16) involves consecutive tensor products, which is paid in term of computer memory. If the \( \gamma_4 \) spectrum (which corresponds to a piece of cubic lattice of size \( 4 \times 4 \times 2 \)) is still very quickly computed, higher sizes turn out to be difficult to reach along this direct track, if only equipped with standard computers memory.

4. Partition function

We now aim to evaluate the partition function

\[ Z = \sum_{\{S_i\}} \exp(-\beta E_{\{S_i\}}), \] (19)

from which all interesting thermodynamical properties can be derived. The reader who has followed the present approach might have already guessed that we shall define a partition function vector \( | Z > \) as:

\[ | Z > = \exp(-\beta | E >) \] (20)

where we use the above defined matrix Hadamard exponential. The standard \( Z \) is simply the sum of \( | Z > \) components. It is again not difficult to derive an iterative relation to get \( | Z_{2N} > \) from \( | Z_N > \), equivalent to expression (16) we had for the spectrum. With the diagonal matrix \( D_{\{Z\}} \) built from \( Z_N \) and \( W_N = \exp(-\beta M_N) \), it reads

\[ \left\{ \begin{array}{l}
| Z_{2N} > = D_{\{Z\}}^{\otimes 2} \text{vec}(W_{2N}) = \text{vec}(D_{\{Z\}} \cdot W_{2N} \cdot D_{\{Z\}}) \\
W_{2N} = W_N \otimes W_N
\end{array} \right. \] (21)

Although quite simple, we detail, in appendix A, the step after step passage from relation (16) to relation (21). The second line of relation (21) arises directly from that of relation (16) upon using relation (16). Quite interestingly, upon additional manipulations, the partition function itself, \( Z_{2N} \), which is the sum of all \( | Z_{2N} > \) elements, simply reads

\[ Z_{2N} = < Z_N | W_{2N} | Z_N > \] (22)

Let us stress that the present approach is different from that followed in ref.\( ^9 \), where the partition function \( Z \) was computed as the inner product of a stabilizer state and a product state, and for the sake of which these authors defined spins living on edges of the graph. In the present case, the square partition function \( Z_4 \) is computed as, with \( x = \exp(-\beta J) \)

\[ Z_4 = (x, x^{-1}, x^{-1}, x) \begin{pmatrix}
x^2 & 1 & 1 & x^{-2} \\
1 & x^2 & x^{-2} & 1 \\
x^{-2} & 1 & x^2 & 1 \\
x^2 & 1 & 1 & x^{-2}
\end{pmatrix} \begin{pmatrix}
x \\
x^{-1} \\
x^{-1} \\
x
\end{pmatrix} = 2(6 + x^4 + x^{-4}) \] (23)
An interesting point arises here. The matrix $W_N$, which encodes the coupling between the two subparts, is diagonalized by a Hadamard matrix (now normalized to have unitary transformations). Indeed, start with the first in the series,

$$W_2 = \begin{pmatrix} x & x^{-1} \\ x^{-1} & x \end{pmatrix}$$

(24)

It is diagonalized under transformation by $H_1$:

$$W'_2 = H_1. W_2. H_1 = \begin{pmatrix} x + x^{-1} & 0 \\ 0 & x - x^{-1} \end{pmatrix} \text{ with now } H_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

(25)

Due to the simple tensor product construction of $W_N$, explicit in the second line of (21), together with the tensor product construction for the Hadamard matrices, the spectrum of $W_N$ is computed directly from that of $W_2$. Recalling that Hadamard matrices square to identity, we can insert the identity matrix on the left and on the right of the square of a partial block-diagonalization. A simple first step, but nevertheless rather trivial, consists in operating a partial block diagonalization has been achieved.

C. Transfer matrices

As already mentionned, the above step by step treatment for the hypercubes also applies, as a one-step procedure, to describe line to line or plane to plane (or graph to graph) addition to form a repeated structure in a given direction. Call $\Lambda_N$ the graph with $N$ vertices to be repeated, and $\Lambda_{2N} = \Lambda_N \cup T(\Lambda_N)$ the resulting graph after one step. We consider the simplest case where each vertex in $\Lambda_N$ has one (translated) neighbour in $T(\Lambda_N)$, suitably numbered as before. The case where each vertex has several new neighbours in the translated copy (as occurs for instance in dense lattices like fcc) could also be treated, with some complications, and will not analysed here. With $|E_N>$ and $|Z_N>$ for the Ising spectum and partition vector for the $\Lambda$ part, relations (16) and (21) still apply to get $|E_{2N}>$ and $|Z_{2N}>$. But, more interestingly, and as expected, the transfer matrix itself is easily derived. $T_N$, the $2^N \times 2^N$ transfer matrix from $\Lambda_N$ to $T(\Lambda_N)$, simply reads :

$$T_N = W_{2N}. D_{|Z|} = W_{2N} \circ |Z_N>$$

(27)

With $m$ copies of $\Lambda$ (and periodic boundary condition) , the partition function follows from the well known trace relation $Z_{mN} = Tr \left(T_N^m \right)$.

While a full diagonalization of $T$ would solve the problem, we shall ask, more modestly, whether Hadamard transformations (with normalized Hadamard matrices from now on) can be helpful to further simplify $T_N$, under the form of a partial block-diagonalization. A simple first step, but nevertheless rather trivial, consists in operating a global Hadamard Transform to the transfer matrix; notice that one should better say an Hadamard conjugation since it reads : $T \rightarrow H^{-1}.T.H$. This leads to split the transfer matrix into two separate blocks, which in fact translates the existence of a global spin-flip symmetry. One could then try to go further and operate with lower order Hadamard matrices on the two blocks. First attempts on small systems show that it might be the case, although no precise conclusions could yet be drawn. As an example, we detail the process in appendix B for the $16 \times 16$ transfer matrix $T_4$ connecting two rings of four spins, which we analyse here in the vanishing $\hbar$ magnetic field limit, and for which a partial block diagonalization has been achieved.

V. CONCLUSION

We have presented a general framework to address Ising-like models on arbitrary graphs. The interactions between spins are neither limited to pairwise interactions, nor restricted to constant couplings. The present approach relies on
a dual structure: a coding state on one side, which represents the interactions carried by the spins, is transformed into a spectral state whose amplitudes are the model energies. The transformation is operated by Hadamard matrices. A main point here is the existence of a Fast Hadamard Transform, which provide therefore potential large speed increase to any numerical computation of the spectrum. But the drawback is its memory consuming part, although sparse vectors enter the game. Whether FHT, sparse algebra and parallelism could be efficiently associated here is an open question addressed to numerical experts.

When the graph is obtained as the union of subgraphs, the proposed analysis simply separates the contribution of the subgraph spectra from that arising from their interaction. Whenever the interaction takes a regular form, we have shown how to compute iteratively the spectrum.

First attempts to compute the partition function and transfer matrices have also been described. Further works need to be done, in particular to check possible transfer matrix block diagonalization algorithms.

Finally, the fact that the Hadamard transform is a main tool for quantum computation raises the question of a possible experimental implementation of the proposed approach.

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VI. SUPPLEMENTARY MATERIALS

A. Derivation of the partition function vector $|Z>$ in expression [21]

As said above, it is not difficult to derive an iterative relation to get $|Z_{2N}\rangle$ from $|Z_N\rangle$, given in expression [21]. It provides nevertheless an interesting exercise to manipulate some of the algebraic tools introduced in the text, and we therefore detail it now, step by step:

$$|Z_{2N}\rangle = \exp (-\beta |E_{2N}\rangle)$$

$$= \exp (-\beta (|E_N\rangle \otimes |E_N\rangle) - \beta \text{vec}(M_{2N}))$$

$$= \exp (-\beta (|E_N\rangle \otimes |E_N\rangle) \circ \text{vec}(M_{2N})) \text{ from (8)}$$

$$= |Z_N\rangle \otimes \text{vec}(W_{2N})$$

$$= D_{2N}^{\otimes 2} \cdot \text{vec}(W_{2N}) \text{ from (8) (Q.E.D.)}$$

$$= \text{vec}(D_Z . W_{2N} . D_Z) \text{ from (11)}$$

The second line of relation [21] arises directly from that of relation [16] upon using relation [10].
B. Partial block diagonalization of the transfer matrix, a simple example.

As announced in the text, we present here the case of the $16 \times 16$ transfer matrix $T_4$ connecting two rings of four spins, which is analysed in the vanishing $h$ magnetic field limit. Using relations \[21\] and \[27\] one easily writes $T_4$ as:

$$T_4 = \begin{pmatrix}
x^8 & x^6 & x^4 & x^6 & x^4 & x^2 & x^6 & x^4 & x^2 & x^2 & 1 \\
x^2 & x^4 & 1 & x^2 & 1 & x^2 & \frac{1}{x^2} & 1 & 1 & x^2 & \frac{1}{x^2} & 1 & 1 & \frac{1}{x^2} & 1 & \frac{1}{x^2} & 1 \\
x^2 & 1 & x^4 & x^2 & 1 & x^2 & 1 & 1 & 1 & x^2 & \frac{1}{x^2} & 1 & 1 & x^2 & \frac{1}{x^2} & 1 & \frac{1}{x^2} & 1 \\
x^2 & 1 & 1 & x^2 & 1 & x^2 & 1 & 1 & 1 & x^2 & \frac{1}{x^2} & 1 & 1 & x^2 & \frac{1}{x^2} & 1 & \frac{1}{x^2} & 1 \\
x^2 & 1 & 1 & 1 & x^2 & 1 & x^2 & 1 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 \\
x^2 & 1 & 1 & 1 & 1 & x^2 & 1 & x^2 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 \\
x^2 & 1 & 1 & 1 & 1 & 1 & x^2 & 1 & x^2 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 \\
x^2 & 1 & 1 & 1 & 1 & 1 & 1 & x^2 & 1 & x^2 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 \\
x^2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & x^2 & 1 & x^2 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 & x^2 & x^4 & 1 \\
\end{pmatrix} \tag{28}$$

A first (trivial) bloc-diagonalization (two $8 \times 8$ blocs), associated with the global spin-flip symmetry, is provided by transforming $T_4$ to $H_4 T_4 H_4$ (recall that $H_4 = H_4^{-1}$ in the normalized case). Combining suitable columns and row permutations, and Hadamard matrices of lower order, one then gets the following spectrum for $T_4$: a set of 8 eigenvalues, shown as pairs (eigenvalue, degeneracy $d$): \{(x^4 - 2 + x^{-4}, d = 4), \left(\left(1 + x^2\right) \left(x^2 - 1\right)^3 / x^4, d = 2\right), \left(\left(1 + x^2\right)^3 \left(x^2 - 1\right) / x^4, d = 2\right)\}; the following two $2 \times 2$ matrices:

$$\begin{pmatrix} x^8 - 1 & 2x^2 \left(x^4 - 1\right) \\ 2x^2 \left(x^4 - 1\right) & x^8 - 1 \end{pmatrix}, \text{ and } \begin{pmatrix} 1 - x^{-8} & \frac{2(x^4 - 1)}{x^2} \\ \frac{2(x^4 - 1)}{x^2} & x^{-8} - \frac{1}{x^4} \end{pmatrix}, \tag{29}$$

and one $4 \times 4$ matrix:

$$\begin{pmatrix} x^8 & 2x^4 & \sqrt{2} \left(x^2 + 2x^4 + x^6\right) & \sqrt{2} \left(-x^2 + 2x^4 - x^6\right) \\ 2x^{-4} & x^{-8} + 1 & \sqrt{2} \left(x^2 + 2x^4 + x^6\right) & \sqrt{2} \left(-x^2 + 2x^4 - x^6\right) \\ 2 + \frac{\sqrt{2}(1+x^2)}{x^2} & 2 + \frac{\sqrt{2}(1+x^2)}{x^2} & x^{-4} + 2\sqrt{2}x^{-2} - 4 + 2\sqrt{2}x^2 + x^4 & -2 \\ 2 - \frac{\sqrt{2}(1+x^2)}{x^2} & 2 - \frac{\sqrt{2}(1+x^2)}{x^2} & -2 & x^{-4} - 2\sqrt{2}x^{-2} + 4 - 2\sqrt{2}x^2 + x^4 \end{pmatrix} \tag{30}$$

These small matrices could again be further simplified, but (apparently) not with Hadamard transforms, so we do not show it. The interested reader can easily recover, from $Tr \left(T_4^4\right)$, the partition function for a $4 \times 4$ square lattice with PBC, whose Ising spectrum was already given in relation \[18\].