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Quantum Monte Carlo scheme for frustrated Heisenberg antiferromagnets

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When one tries to simulate quantum spin systems by the Monte Carlo method, often the "minus-sign problem" is encountered. In such a case, an application of probabilistic methods is not possible. In this paper, the method has been proposed which allows to avoid the minus-sign problem for certain class of frustrated Heisenberg models. The systems where this method is applicable are, for instance, the pyrochlore lattice and the J_1-J_2 Heisenberg model. The method works in singlet sector. It relies on the expression of wave functions in dimer (pseudo)basis and writing down the Hamiltonian as a sum over plaquettes. In such a formulation, matrix elements of the exponent of Hamiltonian are positive.

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I. INTRODUCTION

The systems considered in this paper are Heisenberg models for spin one-half, with competing antiferromagnetic (AF) interactions, i.e., *frustrated* ones:

$$H_\Lambda = \sum_{i,j \in \Lambda} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j,$$

where $\mathbf{s}$ is a vector of Pauli matrices, $\Lambda \subset \mathbb{Z}^d$, $J_{ij} > 0$ (AF case).

Frustrated systems are very interesting and hard to analyze and understand, both in classical version and especially in the quantum case. The source of these difficulties traces back to the large ground-state degeneracy in the classical version. The prototype of such system is an AF Ising model on triangular lattice.[1] Such systems are very sensitive to perturbations. A possible consequence is occurrence of very complicated ground-state and finite temperature phase diagrams. Such a situation has been observed in an ANNNI model[2] (infinite number of phases, devil's staircase, etc). Besides numerous efforts and important results[2–4] (for reviews, see Refs. 5–7), full treatment of such systems is not worked out so far.

The situation for quantum frustrated antiferromagnet is even less clear. It is generally suspected that—in the case of strongly frustrated systems—the ground state emerging as a linear combination of many classical configurations is a featureless, "spin liquid" state, i.e., state without long-range ordering, where correlation functions fall off exponentially.[8] However, one cannot exclude another scenario: "order by disorder"—exotic orderings absent in a classical version of these models. Such scenarios are moreover sensitive to the underlying lattice structure (for a review, see, for instance, Ref. 9). To my best knowledge, no general definite conclusions have been obtained so far.

Among frustrated lattices, perhaps the most popular ones are triangular, kagomé, pyrochlore, and square lattice with "crossing bonds" (called also the J_1-J_2 model). This last case is particularly interesting due to its possible relation with high-temperature superconductivity (HTSC). Quite often, one considers the $t-t'$ two-dimensional Hubbard model as a "minimal model" for HTSC.[10] Behavior of this last model is still not fully understood. A natural starting point in such a study is the limiting case: half-filling and large coupling constant; under these conditions, the $t-t'$ Hubbard model simplifies to J_1-J_2 Heisenberg model.

As a sample of natural questions in the study of frustrated systems, one can mention the following (for definiteness, let us concentrate on the J_1-J_2 Heisenberg model).

(a) Nature of ground state: For which range of values of the ratio $\alpha = J_2/J_1$ we have an antiferromagnetic (Néel) ordering? Is there a spin-liquid state for strong frustration?

(b) Describe the nature of crossover between ordered and disordered states upon increasing frustration.

Exact results on the area of frustrated models are rather rare. For particular forms of interactions, there exist exact results for ground states, obtained by AKLT (Ref. 11) as well as related results.[12] It is, however, unclear if they can be generalized to more general forms of interactions. Some general properties of frustrated systems have been obtained in Refs. 13–15 (they are important in the context of this paper). Moreover, one should mention quite a few approximate reliable results, for instance, Ref. 16 (based on a BCS-like ansatz for wave function).

One of the general tools used to calculate the partition function Z_Λ and thermodynamic functions for quantum spin systems is an application of *Lie-Trotter product formula*. Let us describe the general setup of certain version thereof, i.e., *the Suzuki approach*.[17]

Lie-Trotter product formula[17,18] states that if A,B are finite-dimensional matrices, then

$$e^{A+B} = \lim_{n\to\infty} (e^{A/n} e^{B/n})^n.$$

Using this formula, one calculates Z_Λ in the following way.

(1) Write

$$H = H_1 + H_2,$$

in such a way that H_1,H_2 are sums of *commuting* operators.

(2) Using Lie-Trotter formula, we have

$$Z = \mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr}\, e^{-\beta(H_1+H_2)} = \mathrm{Tr}[\lim_{n\to\infty}(e^{-\beta H_1/n} e^{-\beta H_2/n})^n]$$
$$= \lim_{n\to\infty} \sum_{\{\alpha_1\},\{\alpha_2\},\ldots,\{\alpha_{2n}\}} \langle \alpha_1 | e^{-\beta H_1/n} | \alpha_2 \rangle \times \langle \alpha_2 | e^{-\beta H_2/n} | \alpha_3 \rangle \cdots \langle \alpha_{2n-1} | e^{-\beta H_1/n} | \alpha_{2n} \rangle \langle \alpha_{2n} | e^{-\beta H_2/n} | \alpha_1 \rangle \tag{1}$$

(here $\{\alpha_i\}$ is a basis in the Hilbert space of system states). If it happens that above matrix elements are *positive*, then the life is easier, as one can apply the following *probabilistic* techniques.

(a) Monte Carlo method: in numerical aspects, it is called the quantum Monte Carlo.[19]

(b) Contour expansion techniques[20] or "stochastic geometry" methodology in rigorous studies; as examples, one can mention spin chains,[21] or Bose-Hubbard models.[22,23]

For numerous important cases, matrix elements are positive. It is the case, for instance, of the quantum Ising model in transverse magnetic field, ferromagnetic Heisenberg model, XY model, and Falicov-Kimball model (for a review, see Ref. 19). These systems as well as numerous other ones have been successfully studied with the use of quantum Monte Carlo method.

In general, matrix elements are *not* positive. (This is the famous "minus-sign problem" in the quantum Monte Carlo method.) In certain cases, this problem can be overcome. For instance, if one considers antiferromagnetic Heisenberg model, then for simplest choice of basis states in Eq. (1) (Ising basis), the problem is present. However, it can be overcome for the model on bipartite lattices, using more sophisticated techniques.[24] This is also the case of the Hubbard model on bipartite lattices and for half-filling.[25] Some results for frustrated antiferromagnets have been reported.[26] However, to my best knowledge, the solution of the minus-sign problem is still lacking for general frustrated antiferromagnetic Heisenberg models.

The goal of this paper is elaboration of the quantum Monte Carlo scheme for certain class of frustrated Heisenberg models. Using this scheme, matrix elements obtained are positive.

This scheme concerns the J_1-J_2 Heisenberg model and holds under the following certain conditions.

(1) Presence of reflection symmetry in the system.

(2) We restrict ourselves to the *singlet sector* of the system (i.e., we assume that the total spin of the system is zero).

The first assumption is not too restrictive; it is necessary to apply the Lieb-Schupp theorem (discussed below). The second one is more serious. However, we can argue as follows. For certain class of frustrated antiferromagnetic Heisenberg models (including the pyrochlore and J_1-J_2 model but not the triangular or kagomé lattices), we have Lieb and Schupp theorem[13–15] stating that the ground state of such systems is singlet. One then can hope that performing the Monte Carlo (MC) simulation in the singlet sector at finite temperature T, and then tending with T to zero, we will obtain reliable ground-state properties of such a system.

The sketch of the scheme is as follows. It is well known that positivity of matrix elements is a problem of the choice of basis in the set of "intermediate states" $|\alpha_i\rangle\langle\alpha_i|$ in formula (1) (instructive examples can be found in Ref. 19). If one chooses the basis being a tensor product of Ising states (it is perhaps the simplest choice) as the basis of intermediate states, then some of the matrix elements of Hamiltonian are negative.

Assume, however, that we work in the singlet sector. It is known that every singlet can be built up from *dimers*, i.e. two-spin wave functions of total spin equal to zero. (This will be discussed in Sec. II.) Such a form of singlets has been used in Refs. 8 and 27–29. Consider now the system defined on the $\mathbb{Z}^2$ lattice or, more generally, on a bipartite one (i.e., composed of two sublattices called A and B in such a way that only neighbors of A-type sites are B-type sites and vice versa). Moreover, let us impose the condition that one spin of every dimer belongs to A sublattice and the second one to B sublattice. Now, consider the model with nearest-neighbor (NN) interactions (or, more generally, with unfrustrated ones). It turns out that (for details, see below Sec. III) matrix elements of the Hamiltonian are *non-negative*.

However, if we consider the Heisenberg model with frustrated interactions (for definiteness, take the J_1-J_2 Heisenberg model), then some of the matrix elements are still *negative*. Is it possible to cure this situation? The answer is yes, and the idea is as follows: let us write the Hamiltonian as a sum of the *plaquette* terms, i.e., four-spin Hamiltonians being defined on the 2×2 plaquettes on the lattice. One can hope that in such a situation, negative contributions coming from next-nearest neighbor (NNN) interactions will be compensated by positive ones coming from NN interactions. It turns out that this is the case: matrix elements calculated with the use of plaquettes are positive. The calculations are presented in Sec. IV.

The paper is organized as follows. In Sec. II, the general setup is introduced: construction of singlet wave functions from dimers is explained, and the scalar product of two singlet wave functions is calculated and interpreted in geometrical terms. In Sec. III, the matrix elements of the Hamiltonian written as a sum of two-spin interactions are calculated.

The central part of the paper is Sec. IV, where matrix elements of the Hamiltonian written as a sum of four-spin (plaquette) interactions are calculated. Section V summarizes the results and discusses the possibility of generalizations. In Appendix A, technical tools used in calculations are presented. Appendix B contains (somewhat technical) proof of positivity of matrix elements.

II. DIMERS, SINGLETS, AND ALL THAT

Consider the dimer, i.e., the singlet wave function localized on sites i,j:

$$(ij) = \frac{1}{\sqrt{2}}(|i_+j_-\rangle - |i_-j_+\rangle).$$

Assume now that the total number of spins is even, i.e., we are dealing with $2N$ spin system. Then, every singlet wave function Ψ_{2N} can be built from dimers[27–29]

$$\Psi_{2N} = \sum c_{i_1,\ldots,i_N;j_1,\ldots,j_N}(i_1j_1)(i_2j_2)\ldots(i_Nj_N). \tag{2}$$

This representation is nonunique for $N>1$ (the set of all such dimer products is an overcompleted set of vectors spanning all the space of singlets).

Consider now the *square* lattice. It is a bipartite one, and all considerations below refer also to such lattices. Divide the lattice into two kinds of sites: A- and B-type sites. We demand that in (2),

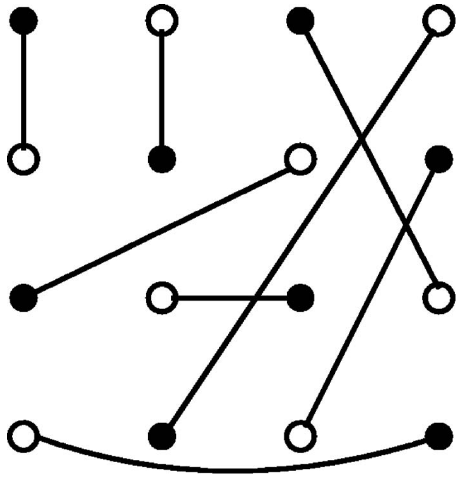

FIG. 1. An example of dimer wave function on 4×4 lattice. Two sorts of sites of the bipartite lattice are represented by circles and heavy dots. Dimers are represented as "bonds" linking lattice sites of opposite kinds.

$$i_k \in A, \quad j_k \in B \quad \text{for all } k=1,\ldots,N. \tag{3}$$

Also, in this case, the set of all dimer products is an overcompleted set (for $N>2$) in the vector space of singlets.[30]

Consider now some singlet wave function on the lattice, which is a product of dimers. Such a function possesses a natural geometric interpretation.[27] Every dimer $(i_k j_k)$ can be illustrated as a "bond" linking lattice sites i_k and j_k (remember $i_k \in A$, $j_k \in B$). Notice that every lattice site is occupied by the end of exactly one bond; in other words, dimers are "closely packed." Such a situation is illustrated in Fig. 1.

Consider now the scalar product of two such functions Ψ_1, Ψ_2:

$$S_{ij} = \langle \Psi_1 | \Psi_2 \rangle. \tag{4}$$

Let us draw both functions on a lattice. Such a situation can be viewed as a set of *closed polygons*. Every such a polygon is formed by dimers belonging to $\Psi_1, \Psi_2, \Psi_1, \Psi_2, \ldots$ (in an alternating manner); the total number of bonds forming this polygon is *even*. It is illustrated in Fig. 2.

Consider first the situation where wave functions Ψ_1,Ψ_2 correspond to *single* nontrivial polygon on the lattice. (We call the polygon nontrivial if it is not a "double bond," i.e., if its length is $2L$, $L>1$.) It is a matter of straightforward calculation (it follows also from the "reduction principle," see below) to show that[27]

$$\langle \Psi_1 | \Psi_2 \rangle = \frac{1}{2^{L-1}}. \tag{5}$$

This result can be generalized to the situation where Ψ_1, Ψ_2 correspond to family of polygons: P_1 of length $2L_1, \ldots;$ P_k of length $2L_k$. In such a case, we have[27]

$$\langle \Psi_1 | \Psi_2 \rangle = 2^{-[\sum_{i=1}^{k} (L_i - 1)]}. \tag{6}$$

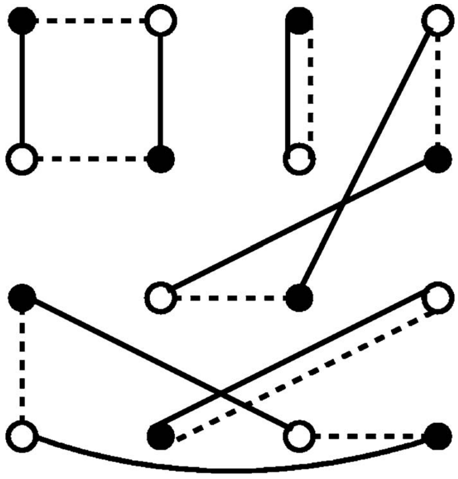

FIG. 2. Two dimer functions (Ψ_1: dashed line and Ψ_2: continuous line) and polygons formed by them. Every site is occupied by exactly one end of dimer belonging to Ψ_1 and the same for Ψ_2. On the picture, there are two trivial polygons (formed by two dimers) and three nontrivial ones (formed by four dimers).

III. MATRIX ELEMENTS OF EXPONENTS OF THE HEISENBERG OPERATOR: TWO-SPIN FORM

In this section, we consider the model with nearest-neighbor interactions. (Although the main interest of this paper are frustrated models, considerations of this section can be treated as a warm-up and a presentation of techniques used in the next section.) The Hamiltonian is of the form

$$H = J \sum_{\langle ij \rangle} h_{ij}, \tag{7}$$

where $h_{ij} = \mathbf{s}_i \cdot \mathbf{s}_j$.

Write expression (7) in the form

$$H = H_1 + H_2 + H_3 + H_4, \tag{8}$$

in such a way that $H_1, \ldots, H_4$ are sums of commuting operators. One possible way to achieve this goal is as follows. Every site index i is, in fact, a two-index: $i=(i_x,i_y)$, where i_x is the horizontal index on the lattice and i_y is the vertical index. Divide the Hamiltonian (7) into $H_1, \ldots, H_4$ in the following way.

(a) H_1 is a sum of these operators h_{ij}, where i,j are of the form: $(2k,2l),(2k,2l+1)$. Denote it as type 1.

(b) H_2 is a sum of h_{ij}'s, where i,j are of the form $(2k,2l),(2k+1,2l)$, type 2.

(c) H_3 is a sum of h_{ij}'s, where i,j are of the form $(2k,2l+1),(2k+1,2l+1)$, type 3.

(d) H_4 is a sum of h_{ij}'s, where i,j are of the form $(2k+l,2l),(2k+1,2l+1)$, type 4.

In the left-hand side of formula (1), it is sufficient to take trace over singlet states only. However, what about the right-hand side, where we have sum over all intermediate states? It turns out that it is also sufficient to take all intermediate states in the singlet sector only. It is so because all Hamiltonians $H_1, \ldots, H_4$ commute with total spin operator. It implies that "intersector" matrix elements are zero.

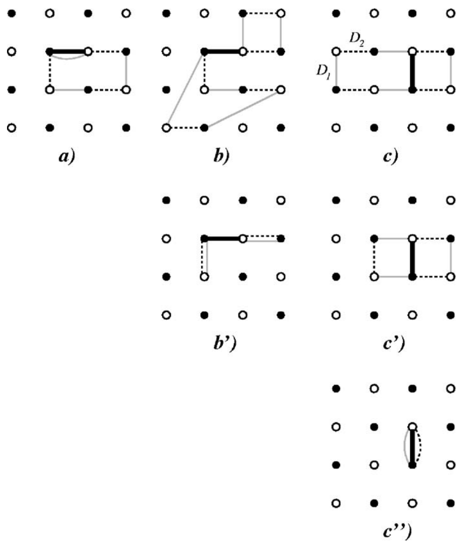

FIG. 3. (a)–(c) Three kinds of matrix elements of the operator $\exp(Kh_{ij})$ listed above. The action of this operator is denoted as a bold line; gray and dashed lines denote dimers forming the functions Ψ_1 and Ψ_2, respectively. (c′) is obtained from (c) by one step of reduction principle (R.I); upon this operation, neighboring dimers D_1 and D_2 are eliminated. (b′) is obtained from (b) by three steps of reduction (R.I.) (c″) has been obtained from (c′) by two steps of (R.II).

Consider now a matrix element $\langle\Psi_I|\exp(KH_k)|\Psi_J\rangle$, $k=1,\ldots,4$ in order to check its positivity. Every operator H_k is a sum of commuting operators; so, if $H_k=\Sigma_{i,j \text{ of type } k}h_{ij}$, then $\exp(KH_k)=\Pi_{i,j \text{ of type } k}\exp(Kh_{ij})$ and one can write

$$\langle\Psi_I|\exp(KH_k)|\Psi_J\rangle = \sum_{\alpha_1}\sum_{\alpha_2}\cdots\sum_{\alpha_M}\langle\Psi_I|\exp(Kh_{i_1j_1})|\Psi_{\alpha_1}\rangle \times\langle\Psi_{\alpha_1}|\exp(Kh_{i_2j_2})|\Psi_{\alpha_2}\rangle\ldots\langle\Psi_{\alpha_M}|\exp(Kh_{i_Mj_M})\Psi_J\rangle$$

(here M is a number of operators h_{ij} in H_k). We can make a conclusion that if matrix elements of the operator $\exp(Kh_{ij})$ are positive, then the matrix element of $\exp(KH_k)$ is also positive.

Let us calculate the matrix element of the two-spin operator h_{ij}:

$$\langle\Psi_1|\exp(Kh_{ij})|\Psi_2\rangle, \tag{9}$$

where $|\Psi_1\rangle,|\Psi_2\rangle$ are dimer functions, and $K=-\beta J/N$. Notice that antiferromagnetic case $J>0$ imply $K\in]-\infty,0[$.

Below, the following notation will be useful:

$$\epsilon^1=\exp(K/2), \quad \epsilon_3=\exp(-3K/2).$$

Notice that $\epsilon^1\in]0,1[$, $\epsilon_3\in]1,\infty[$.

Let us consider first the situation where i,j are nearest neighbors. We have three sorts of situation.

(a) The operator $\exp(Kh_{ij})$ acts on $|\Psi_1\rangle$, which contains the (ij) dimer; it is illustrated in Fig. 3(a). The value of the matrix element is

$$\langle\Psi_2|\exp(Kh_{ij})|\Psi_1\rangle=\epsilon_3\langle\Psi_2|\Psi_1\rangle, \tag{10}$$

we see that this element is positive.

(b) The operator $\exp(Kh_{ij})$ is localized on a bond connecting two different polygons, see Fig. 3(b). We have

$$\langle\Psi_2|\exp(Kh_{ij})|\Psi_1\rangle=\frac{1}{4}(3\epsilon^1+\epsilon_3)\langle\Psi_2|\Psi_1\rangle, \tag{11}$$

which is also positive.

(c) The operator $\exp(Kh_{ij})$ acts inside one connected polygon, but there are at least three polygon bonds between i and j sites, see Fig. 3(c). In such a situation, we have

$$\langle\Psi_2|\exp(Kh_{ij})|\Psi_1\rangle=\epsilon_3\langle\Psi_2|\Psi_1\rangle, \tag{12}$$

clearly, it is also positive.

Similar matrix elements (but of the operator h_{ij} instead of its exponent) have been calculated in Ref. 27. In the case considered here, they have been derived by straightforward calculation with the use of simple algebraic tools: spectral resolution of the operator h_{ij} and the reduction principle. Details of calculation of matrix elements are presented below.

A matrix element for situation (a) [presented in Fig. 3(a)] can be calculated immediately. Namely, in this situation, the operator $\exp(Kh_{ij})$ acts for dimer function (ij), which is an *eigenfunction* of h_{ij} [and of course of $\exp(Kh_{ij})$]. Using property (A3), we get expression (10).

For situations (b) and (c) [presented in Figs. 3(b) and 3(c)], we apply the *reduction principle* first. Such a reduction is performed in two steps, (R.I) and (R.II).

(R.I) We examine the quotient q:

$$q=\frac{\langle\Psi_2|\exp(Kh_{ij})|\Psi_1\rangle}{\langle\Psi_2|\Psi_1\rangle}, \tag{13}$$

where Ψ_1 and Ψ_2 functions form closed (not necessarily connected) polygon P. Assume that these functions can be written as $\Psi_1=\Phi_1(lk)(nm)$, $\Psi_2=\Phi_2(lm)(np)$. Let us remove the site l and identify k and m sites [this situation can be viewed as removing dimers $D_1=(kl)$ from Ψ_1 and $D_2=(mk)$ from Ψ_2 with subsequent identifications of sites k and m]. This way, we obtain "reduced" functions $\Psi_1^R=\Phi_1(nk)$ and $\Psi_2^R=\Phi_2(np)$ and reduced polygon P^R. We assume that all sites k, l, m, n, and p are at a distance greater than 1 from i and j. Then, the quotient q obtained for functions Ψ_1 and Ψ_2 (13) is equal to the quotient q^R calculated for functions Ψ_1^R and Ψ_2^R:

$$q^R=\frac{\langle\Psi_2^R|\exp(Kh_{ij})|\Psi_1^R\rangle}{\langle\Psi_2^R|\Psi_1^R\rangle}. \tag{14}$$

Expressing the result in a less formal manner, we can say that the quotient q will not change if we remove two neighboring dimers from the polygon P.

Proof. Let us remember how to calculate the scalar product for dimer wave functions: After expressing them in the "plus-minus" basis, we sum over all sites and spin degrees of freedom for every site.

Let us consider the matrix element $\langle\Psi_2|\exp(Kh_{ij})|\Psi_1\rangle$. Let us expand dimer functions (lk), (nm), (lm), and (np) in the base of plus-minus functions. Then, let us sum over spin indices of sites l and m. After straightforward calculations, remembering about normalization factors for dimers and using orthonormality relation of spin functions on arbitrary site r: $\langle r_\sigma|r_{\sigma'}\rangle=\delta_{\sigma\sigma'}$, we obtain

$$\langle\Psi_2|\exp(Kh_{ij})|\Psi_1\rangle = \frac{1}{2}\langle\Psi_2^R|\exp(Kh_{ij})|\Psi_1^R\rangle. \tag{15}$$

Analogous calculation gives

$$\langle\Psi_2|\Psi_1\rangle = \frac{1}{2}\langle\Psi_2^R|\Psi_1^R\rangle, \tag{16}$$

so we obtain desired equality $q=q_R$.

After (possibly, multiple) application of reduction principle to situations as in Figs. 3(b) and 3(c), we get situations such as in Figs. 3(b′) and 3(c′). This way, reduction principle simplifies the calculation of matrix elements to the case, where wave functions occupy at most six sites.

(R.II) By straightforward calculation, one obtains that both cases illustrated in Figs. 3(c′) and 3(c″) give an equal value of q. (This step is not necessary, but its analogon for plaquettes will be useful due to economy reasons.)

Two cases obtained after reduction, i.e., the ones illustrated in Figs. 3(b′) and 3(c′) [or, equivalently, Fig. 3(c″)], can be calculated immediately. The line of calculations is as follows: for the wave function Ψ_1, one passes from dimer form to the plus-minus basis. Then, one calculates an action of the operator $\exp(Kh_{ij})$ on Ψ_1, making use of the spectral resolution of the operator h_{ij} given by Eqs. (A4) and (A5) as well as formula (A3). Finally, one calculates the scalar product of expression obtained with the Ψ_2 function, expressed in the plus-minus basis.

We can conclude this section by the statement that matrix elements for nearest-neighbor Heisenberg model are positive, so we have no minus-sign problem here. In my opinion, such a result can be viewed as an interesting one, but not exciting: There are other approaches, where minus-sign problem has been overcome.[24–26]

Now, let us consider the frustrated case (i.e., the J_1-J_2 Heisenberg model). In this case, however, the matrix elements are in general *not positive*. As an example, let us mention situation analogous to the case (b) above, but where i,j are next-nearest neighbors. In such a case, we have

$$\langle\Psi_2|\exp(Kh_{ij})|\Psi_1\rangle = -\frac{1}{4}(3\epsilon^1+\epsilon_3)\langle\Psi_2|\Psi_1\rangle, \tag{17}$$

which is not positive. In other words, for frustrated (J_1-J_2) model, where both NN and NNN interactions are present, the minus-sign problem still exists.

How to cure the problem? The idea is as follows: write the Hamiltonian as a sum over *plaquettes* (four-spin) sets. One can hope that negative contribution will be compensated by positive one. (It is not obvious *a priori*, as two-body operators entering into plaquette operator do not commute, in general.) It turns out that in such a formulation, the matrix elements are positive; details are described in the following section.

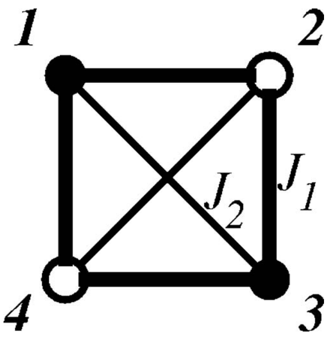

FIG. 4. Elementary plaquette on which the plaquette Hamiltonian (18) is defined. Sites are arranged clockwise.

IV. MATRIX ELEMENTS OF EXPONENTS OF THE HEISENBERG OPERATOR: PLAQUETTE FORM

Consider the Heisenberg model on a (subset of) square lattice. We assume that there are NN and NNN interactions. For the sake of concreteness, we consider the J_1-J_2 model, but all considerations also apply in the case of "pyrochlore" lattice and some others. We assume that the system exhibits the reflection symmetry as in such a case; the ground state is a singlet.

Remark. In Refs. 14 and 31, it has been proven that the ground state is singlet for $J_2/J_1\leq 1$, where J_1,J_2 are coupling constants defined *on a plaquette*. When the Hamiltonian of the full system with periodic boundary conditions is expressed as a sum of two-site interactions, this condition should be rewritten in the form $j_2/j_1\leq 1/2$, where j_1 is the NN interaction and j_2 is the NNN interaction.

The setup for wave functions is the same as previously: We assume that wave functions are built up from "bipartite" dimers. Consider the Hamiltonian defined on a square plaquette:

$$h_\Box = h_{12}+h_{23}+h_{34}+h_{41}+\alpha(h_{13}+h_{24}), \tag{18}$$

(see Fig. 4), where $h_{ij}=\mathbf{s}_i\cdot\mathbf{s}_j$, $\alpha=J_2/J_1$.

We have

$$H=\sum_{i\in\Lambda} h_{\Box,i}. \tag{19}$$

Analogously as before, let us write the Hamiltonian in the form

$$H=H_1+H_2+H_3+H_4, \tag{20}$$

where each of terms $H_1,\ldots,H_4$ is a sum of commuting plaquette operators. This division can be done, for instance, in the following form. Plaquette index in Eq. (19) is, in fact, a two-index: $i=(i_x,i_y)$, where i_x horizontal component and i_y is the vertical one. $H_1,\ldots,H_4$ are defined as is the follows.

(a) H_1 is a sum of these operators $h_{\Box,i}$, where i is of the form $(2k,2l)$. Denote it as type 1.

(b) H_2 is a sum of these operators $h_{\Box,i}$, where i is of the form $(2k+1,2l)$. Denote it as type 2.

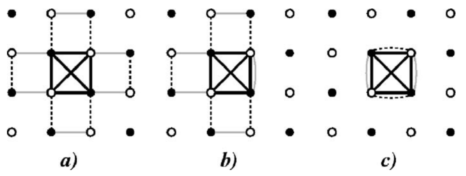

FIG. 5. Illustration of the action (R.II.plaq). (a) corresponds to initial configuration, (b) illustrates the configuration after single action of (R.II.plaq), and (c) is the picture after three further subsequent actions of (R.II.plaq). All three configurations have the same value of $q_{\square}$.

(c) H_3 is a sum of these operators $h_{\square,i}$, where i is of the form $(2k,2l+1)$. Denote it as type 3.

(d) H_4 is a sum of these operators $h_{\square,i}$, where i is of the form $(2k+1,2l+1)$. Denote it as type 4.

As in the previous section, one shows that if matrix elements of elementary plaquette operator $\langle\Psi_I|\exp(Kh_{\square})|\Psi_J\rangle$ are positive, then matrix elements $\langle\Psi_I|\exp(KH_k)|\Psi_J\rangle$ are also positive. Let us calculate the matrix element of $h_{\square}$. This will be done in two stages. In the first step, we apply the reduction principle. Its first stage (R.I.plaq) is identical as in the case of two-site Hamiltonian (R.I), i.e., it allows to decrease the number of neighboring polygon edges by 2 without change of the quotient $q_{\square}$, where $q_{\square}$ is

$$q_{\square}=\frac{\langle\Psi_2|\exp(Kh_{\square})|\Psi_1\rangle}{\langle\Psi_2|\Psi_1\rangle}. \tag{21}$$

The proof of (R.I.plaq) is also identical as previously, so we will not repeat it. This way, all calculations are reduced to cases where wave functions occupy at most 12 sites. It is possible further reduction. This second step of reduction is similar to (R.II) but not identical.

(R.II.plaq): Assume that in the configuration there appear a square consisting of the following sides: one edge belongs to the Hamiltonian plaquette [say, this is (i,j) side], two sides are dimers belonging to the function Ψ_1: (i,l), (k,j), and the last side is dimer belonging to the function Ψ_2: let it be (k,l). In such a configuration, one can eliminate two sides (k,j) and (k,l) and replace the square (i,j,k,l) by one bond (i,j) with dimer (i,j).

The proof of (R.II.plaq) can be obtained by a straightforward calculation. An example of its action is illustrated in Fig. 5. This way, after reductions, we have to calculate matrix elements of the plaquette Hamiltonian with wave functions defined on at most eight sites.

It turns out that there are eight such configurations. They are illustrated in Fig. 6. The matrix elements corresponding to them can be calculated in a straightforward manner, similarly as in the previous section for the case of two-spin Hamiltonian. Basic steps of such calculations are the following.

(1) We express dimer functions in the plus-minus basis.

(2) We calculate the action of the $\exp(Kh_{\square})$ operator on the function Ψ_1, using the spectral resolution of the operator $h_{\square}$ (necessary formulas are collected in Appendix A 2) together with the formula (A3).

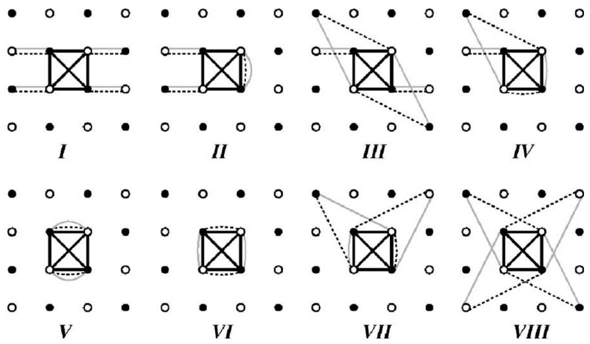

FIG. 6. Reduced configurations for plaquette Hamiltonian.

(3) In the last step, we calculate the scalar product of the expression obtained above with the wave function Ψ_2 (expressed in the plus-minus basis).

Calculations are straightforward but lengthy, and they have been performed with the use of symbolic calculation program (MAPLE). The results are summarized in Table I below.

In formulas below, the following notation has been used $y=\exp(-K)$; $a=\alpha/2$. We assume that $0\leqslant\alpha\leqslant 1$ (as for these values of α, we have warranty that the ground state of the system is singlet[15,31]). Remember that for $0\leqslant T\leqslant\infty$, we have $1\leqslant y\leqslant\infty$.

Some of the expressions in the table are evidently positive (there are I, II, and V). It turns out that remaining expressions are also positive. However, these considerations are rather technical and have been relegated to Appendix A 2. Let us summarize this section by the statement that in the dimer basis, and for the Hamiltonian written as a sum of plaquettes, matrix elements of the $\exp(Kh_{\square})$ are positive.

V. SUMMARY AND CONCLUSIONS

The technical tool to study (certain class of) frustrated systems has been developed, which (hopefully) would allow

TABLE I. Values of matrix elements of the quotient $q_{\square}$ for eight reduced configurations in Fig. 6.

No.	$q_{\square}$
I	$\frac{1}{16}(y^{3a}+y^{2-a}+6y^{a}+3y^{1-a}+5y^{-1-a})$
II	$\frac{1}{16}(y^{3a}+3y^{2-a}+6y^{a}+6y^{1-a})$
III	$\frac{1}{8}(-y^{3a}+y^{2-a}+3y^{1-a}+5y^{-1-a})$
IV	$\frac{1}{8}(-y^{3a}+3y^{2-a}+6y^{1-a})$
V	$\frac{1}{4}(y^{3a}+3y^{2-a})$
VI	$\frac{1}{2}(-y^{3a}+3y^{2-a})$
VII	$\frac{1}{4}(y^{3a}+3y^{2-a}-6y^{a}+6y^{1-a})$
VIII	$\frac{1}{4}(y^{3a}+y^{2-a}-6y^{a}+3y^{1-a}+5y^{-1-a})$

application of probabilistic techniques. This paper is devoted to the J_1-J_2 Heisenberg model in any dimension (and models whose Hamiltonians are sums of frustrated plaquette Hamiltonians; the pyrochlore lattice is perhaps the most typical example). It would be tempting to generalize the method to other frustrated systems. Such a generalization probably can be realized in the case of other systems exhibiting reflection symmetry, for instance, three-dimensional Heisenberg models with frustrated cubes; of course, one have to check the positivity of the matrix elements of Hamiltonians for frustrated units.

Generalization for frustrated systems exhibiting no reflection symmetry (such as kagomé or triangular ones in two dimensions) is less obvious. For such systems, matrix elements of frustrated units can be positive (author calculated such elements for triangular lattice and positivity holds also in this case). However, on the other hand, the method relies heavily on the assumption that we are working in the singlet sector. It has been proved that the ground state(s) of the J_1-J_2 Heisenberg model is (one) singlet,[13–15,31] but for triangular or kagomé lattices, it is not proved. (The answer is probably positive, but the proof—as far I know—is lacking.) If the ground state is singlet, then also in the case of a triangular lattice, one can try to simulate the ground state using this method.

The next point is the technical one: full Monte Carlo simulation of dimerlike models is rather a difficult task.[32] It is not clear how difficult would be an implementation of the actual method; this paper is devoted only to development of the scheme. However, certain attempts toward concrete computational realization of this method are in progress. These attempts are based on certain simplified version of the Monte Carlo method, which can be called "ansatz Monte Carlo" and has been developed, among others, in Ref. 27.

It would be interesting to try to develop analogous method in the sector of S arbitrary, not only $S=0$. If successful, it would be possible to perform quantum MC simulations in arbitrary temperatures, not only in low-region (as in the present version). Moreover, it would also be possible to simulate systems where there is no warranty that the ground state is singlet. There are some indications that the procedure described in this paper could be generalized for S arbitrary. However, at this moment, it is too early to say something definite.

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APPENDIX A: TECHNIQUES USED IN CALCULATION OF MATRIX ELEMENTS

Let A be the self-adjoint operator in finite-dimensional Hilbert space $\mathcal{H}$, $\dim \mathcal{H}=N$; let $\mathrm{Sp}(A)=\{\lambda_i\}$—spectrum of A, V_i—the subspace corresponding to the eigenvalue λ_i, $\dim V_i=n_i$. We have $\Sigma_i n_i=N$, $\mathcal{H}=\oplus_i V_i$. Every such operator A can be represented in the form of the *spectral resolution*

$$A=\sum_i \lambda_i P_i, \tag{A1}$$

where P_i is the orthogonal projection onto corresponding subspace V_i. These projections possess well-known properties: $\Sigma_i P_i = Id_{\mathcal{H}}$ ($Id_{\mathcal{H}}$ is the identity operator in $\mathcal{H}$); $P_i^2=P_i$ for every i; $P_iP_j=P_jP_i=0$ for $i\neq j$. Every such projection P_i onto eigensubspace V_i can be calculated from the famous formula

$$P_i=\sum_{k=1}^{n_i} |v_{i_k}\rangle\langle v_{i_k}|, \tag{A2}$$

where $|v_{i_k}\rangle$ is the kth vector of orthonormal base spanning the V_i subspace.

If $f(x)$ is an analytic function, then we have

$$f(A)=\sum_i f(\lambda_i)P_i. \tag{A3}$$

For the sake of completeness, we present below expressions for projections, which appear in the spectral resolutions of operators h_{ij} and $h_\square$.

1. Spectral resolution of the operator h_{ij}

For two spins, the state space $\mathcal{H}_2$ is four dimensional. The Hamiltonian $h_{ij}=\mathbf{s}_i\cdot\mathbf{s}_j$ commutes with the total spin operator, so eigenvalues of h_{ij} can be classified according to angular momentum quantum numbers. Eigenvalues of h_{ij} are $E_0=-\frac{3}{4}$ (total spin S is zero, i.e., the state is singlet; its multiplicity is 1) and $E_1=\frac{1}{4}$ (here, total spin S is 1, i.e., it is a triplet. We have three triplet states with zth component of angular momentum equal to $+1,0,-1$; all of them have the same energy, so the multiplicity of E_1 is 3).

Let us choose in $\mathcal{H}_2$ the standard (plus-minus) basis $e_1,\ldots,e_4$:

$$e_1=|i_+j_+\rangle,\quad e_2=|i_+j_-\rangle,\quad e_3=|i_-j_+\rangle,\quad e_4=|i_-j_-\rangle.$$

In this basis, the Hamiltonian h_{ij} is given by the matrix

$$h_{ij}=\mathbf{s}_i\cdot\mathbf{s}_j=\frac{1}{4}\begin{bmatrix}1&0&0&0\\0&-1&2&0\\0&2&-1&0\\0&0&0&1\end{bmatrix}. \tag{A4}$$

Projectors P_0 (onto singlet subspace) and P_1 (onto triplet subspace) are

$$P_0=\frac{1}{2}\begin{bmatrix}0&0&0&0\\0&1&-1&0\\0&-1&1&0\\0&0&0&0\end{bmatrix},\quad P_1=\frac{1}{2}\begin{bmatrix}2&0&0&0\\0&1&1&0\\0&1&1&0\\0&0&0&2\end{bmatrix}. \tag{A5}$$

2. Spectral resolution of the operator $h_\square$

The space of states for the system of four spins $\mathcal{H}_4$ is $2^4=16$ dimensional. In such a situation, it is again very useful to exploit properties of the angular momentum operator and classify states according to spin quantum numbers.

The plaquette Hamiltonian is given by Eq. (18). Remember $\alpha=J_2/J_1$; it is more convenient to introduce $a=\alpha/2$. The Hamiltonian (18) commutes with total angular momentum operator **S**. For eigenstates and eigenvalues of the Hamiltonian, good quantum numbers are S (total spin) and M (zth component of spin). Let us classify states according to the value of M first, and then, in every sector with given M, classify the states according to S. For each such state, we will give their energies and corresponding projectors. Classification of states with respect to values of M proceeds as follows.

Among all 16 states, we have the following.

(a) One state with $M=2$ (plus twin state $M=-2$). Both of them share $S=2$.

(b) Four states with $M=1$. Among them, there are one state $S=2$, $M=1$ and three states $S=1$, $M=1$. There are also twin states for $M=-1$.

(c) Six $M=0$ states. There are one state $S=2$, $M=0$; three states $S=1$, $M=0$; and two states $S=0$, $M=0$.

We can consider only states with non-negative values of M, as all of them possess their twins for $-M$.

Consider now all M sectors. Eigenvalues will be denoted as $E^{(n)}_{S,M}$ (n is the index of the state) and corresponding projections by $P^{(n)}_{S,M}$.

$M=2$ *sector*. This is subspace spanned by one base vector

$$e^{(2)}_1=\left|\begin{matrix} + & + \\ + & + \end{matrix}\right\rangle .$$

The Hamiltonian in this sector is simply a number $1+a$, which is of course also the eigenvalue $E^{(1)}_{2,2}$. The projection is trivial.

$M=1$ *sector*. This subspace is four dimensional. As a basis, let us choose

$$e^{(1)}_1=\left|\begin{matrix} - & + \\ + & + \end{matrix}\right\rangle ,$$

$$e^{(1)}_2=\left|\begin{matrix} + & - \\ + & + \end{matrix}\right\rangle ,\quad e^{(1)}_3=\left|\begin{matrix} + & + \\ - & + \end{matrix}\right\rangle ,\quad e^{(1)}_4=\left|\begin{matrix} + & + \\ + & - \end{matrix}\right\rangle . \tag{A6}$$

The Hamiltonian in this basis is given by

$$h_\square=\frac{1}{2}\begin{bmatrix} 0 & 1 & 2a & 1 \\ 1 & 0 & 1 & 2a \\ 2a & 1 & 0 & 1 \\ 1 & 2a & 1 & 0 \end{bmatrix}. \tag{A7}$$

Eigenvalues (i.e., energies) and corresponding projectors are

$$E^{(1)}_{2,1}=1+a,\quad P^{(1)}_{2,1}=\frac{1}{4}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

(this is $M=1$ component of quintet). The remaining three states are triplets (more precisely, the $M=1$ components thereof). Two of them are degenerate: the subspace spanned by eigenvectors of $E^{(1)}_{1,1}$ is two dimensional:

$$E^{(1)}_{1,1}=-a,\quad P^{(1)}_{1,1}=\frac{1}{2}\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix},$$

$$E^{(2)}_{1,1}=-1+a,\quad P^{(2)}_{1,1}=\frac{1}{4}\begin{bmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{bmatrix}.$$

Finally, consider the $M=0$ sector. The basis is

$$e^{(0)}_1=\left|\begin{matrix} + & + \\ - & - \end{matrix}\right\rangle ,$$

$$e^{(0)}_2=\left|\begin{matrix} - & - \\ + & + \end{matrix}\right\rangle ,\quad e^{(0)}_3=\left|\begin{matrix} + & - \\ + & - \end{matrix}\right\rangle ,\quad e^{(0)}_4=\left|\begin{matrix} - & + \\ - & + \end{matrix}\right\rangle ,$$

$$e^{(0)}_5=\left|\begin{matrix} + & - \\ - & + \end{matrix}\right\rangle ,\quad e^{(0)}_6=\left|\begin{matrix} - & + \\ + & - \end{matrix}\right\rangle . \tag{A8}$$

The Hamiltonian in $M=0$ sector is

$$h=\frac{1}{2}\begin{bmatrix} -2a & 0 & 2a & 2a & 1 & 1 \\ 0 & -2a & 2a & 2a & 1 & 1 \\ 2a & 2a & -2a & 0 & 1 & 1 \\ 2a & 2a & 0 & -2a & 1 & 1 \\ 1 & 1 & 1 & 1 & -2+2a & 0 \\ 1 & 1 & 1 & 1 & 0 & -2+2a \end{bmatrix}. \tag{A9}$$

Eigenvalues and projectors are as follows.

The $M=0$ component of quintet:

$$E^{(1)}_{2,0}=1+a,\quad P^{(1)}_{2,0}=\frac{1}{6}\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}. \tag{A10}$$

The $M=0$ components of triplets:

$$E_{1,0}^{(1)} = -a, \quad P_{1,0}^{(1)} = \frac{1}{2}\begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{A11}$$

[remember that subspace spanned by eigenvectors corresponding to $E_{1,0}^{(1)}$ is two dimensional], and

$$E_{1,0}^{(2)} = -1 + a, \quad P_{1,0}^{(2)} = \frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}. \tag{A12}$$

Finally, the $M=0$ components of singlets:

$$E_{0,0}^{(1)} = -3a, \quad P_{0,0}^{(1)} = \frac{1}{4}\begin{bmatrix} 1 & 1 & -1 & -1 & 0 & 0 \\ 1 & 1 & -1 & -1 & 0 & 0 \\ -1 & -1 & 1 & 1 & 0 & 0 \\ -1 & -1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \tag{A13}$$

$$E_{0,0}^{(2)} = -2 + a, \quad P_{0,0}^{(2)} = \frac{1}{12}\begin{bmatrix} 1 & 1 & 1 & 1 & -2 & -2 \\ 1 & 1 & 1 & 1 & -2 & -2 \\ 1 & 1 & 1 & 1 & -2 & -2 \\ 1 & 1 & 1 & 1 & -2 & -2 \\ -2 & -2 & -2 & -2 & 4 & 4 \\ -2 & -2 & -2 & -2 & 4 & 4 \end{bmatrix}. \tag{A14}$$

APPENDIX B: POSITIVITY OF MATRIX ELEMENTS FOR PLAQUETTE HAMILTONIAN

In this appendix, positivity of matrix elements in the table in Sec. IV is proven. Remember that $a \in [0, \frac{1}{2}]$ and $y \in [1, \infty]$. Factors before expressions for $q_\Box$ are skipped.

In situation III, we have

$$-y^{3a} + y^{2-a} + 3y^{1-a} + 5y^{-1-a} \geqslant -y^{3a} + y^{2-a} = y^{3a}(-1 + y^{2-4a}),$$

but for $2-4a \geqslant 0$ and for $y > 1$, we have $(-1+y^{2-4a}) > 0$.

In situation IV, we have

$$-y^{3a} + 3y^{2-a} + 6y^{1-a} \geqslant -y^{3a} + y^{2-a},$$

and this is the same expression as in situation III.

In situation VI, we have

$$-y^{3a} + 3y^{2-a} \geqslant -y^{3a} + y^{2-a},$$

so we again obtain case studied in situation III.

In situation VII, we have

$$y^{3a} + 3y^{2-a} - 6y^{a} + 6y^{1-a} \geqslant 6(-y^{a} + y^{1-a}) = 6y^{a}(-1 + y^{1-2a})$$

and, analogously as in situation III, conditions $1-2a \geqslant 0$, $y > 1$ imply that $-1+y^{1-2a} > 0$.

Situation VIII. This is the most complicated one. Write first

$$y^{3a} + y^{2-a} - 6y^{a} + 3y^{1-a} + 5y^{-1-a} = y^{3a} + y^{2-a} - 3y^{a} + 5y^{-1-a} + 3(-y^{a} + y^{1-a}).$$

Due to argumentation identical as in situation III, the last term (in parentheses) is positive: $-y^{a}+y^{1-a}=y^{a}(-1+y^{1-2a}) \geqslant 0$. So, it is sufficient to show positivity of $y^{3a}+y^{2-a}-3y^{a}+5y^{-1-a}=y^{a}(y^{2a}+y^{2-2a}-3+5y^{-1-2a})$. Consider two extreme cases (i.e., $a=0$ and $a=\frac{1}{2}$) of the expression in parentheses above. We have for $a=0$:

$$1 + y^{2} - 3 + 5y^{-1} > y - 2 + \frac{1}{y} + \frac{4}{y} = \left(\sqrt{y} - \frac{1}{\sqrt{y}}\right)^{2} + \frac{4}{y} > 0,$$

and for $a=\frac{1}{2}$,

$$y + y - 3 + 5y^{-2} = y^{-2}(2y^{3} - 3y^{2} + 5) = y^{-2}(y + 1)(2y^{2} - 5y + 5),$$

which is greater than zero for $y \geqslant 1$, as it follows from elementary considerations. For intermediate values of a, i.e., $0 < a < \frac{1}{2}$, let us write $y^{2a}+y^{2-2a}-3+5y^{-1-2a}=y^{-1-2a}(y^{1+4a}+y^{3}-3y^{1+2a}+5)$ and notice that $y^{1+4a} > y$, $-y^{1+2a} > -y^{2}$, so we have $y^{1+4a}+y^{3}-3y^{1+2a}+5 > y+y^{3}-3y^{2}+5=(y+1)(y^{2}-4y+5) > 0$, thus establishing positivity of VIII.

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