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Compression of Hamiltonian matrix: Application to spin-1/2 Heisenberg square lattice

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We introduce a simple algorithm providing a compressed representation ($\in \mathbb{R}^{N_{\text{orbits}} \times N_{\text{orbits}}} \times \mathbb{N}^{N_{\text{orbits}}}$) of an irreducible Hamiltonian matrix (number of magnons M constrained, dimension: $\frac{N_{\text{spins}}!}{M!(N_{\text{spins}}-M)!} > N_{\text{orbits}}$) of the spin-1/2 Heisenberg anti-ferromagnet on the $L \times L$ non-periodic lattice, not looking for a good basis. As L increases, the ratio of the matrix dimension to N_{orbits} converges to 8 (order of the symmetry group of square) for the exact ground state computation. The sparsity of the Hamiltonian is retained in the compressed representation. Thus, the computational time and memory consumptions are reduced in proportion to the ratio. © 2016 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>). [<http://dx.doi.org/10.1063/1.4963834>]

I. INTRODUCTION

In mathematics, a matrix is irreducible if it is not similar via a permutation to a block upper triangular matrix.¹ Graph-theoretically, replacing non-zero entries in the matrix by one, and viewing the matrix as the adjacency matrix of a directed graph, the matrix is irreducible if and only if such directed graph is strongly connected.² If a symmetric structure is inherent in such an irreducible matrix, there is a block-diagonalized similar matrix having the same eigenvalues.³ Once we construct the bases of various irreducible subspaces, low-rank matrices can be obtained, which allow us to compute all the eigenpairs.

Frequently, it takes a great deal of effort and time to search for a good basis block-diagonalizing such an irreducible matrix and calculate new matrix elements. In quantum chemistry, generating matrix elements of a Hamiltonian by itself is often the most time consuming part.⁴ In addition, such low-rank matrices are not as sparse as original irreducible matrix in general; they could be even denser. For instance, the ground state energy of the 8-site Heisenberg spin-1/2 cube (matrix dimension: $2^8 = 256$) can be obtained from an irreducible matrix of rank 70 (number of magnons constrained to be 4) or such a low-rank block (dimension: 6) after a change of basis. In contrast to the original Hamiltonian and the irreducible matrix (sparse matrices), however, the low-rank block is now the following dense matrix (numerically represented):⁵

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$$\begin{bmatrix} 0 & 0.8666 & 0.8666 & 0 & 0 & 0 \\ 0.8666 & -1.5 & 0.5000 & 0.5000 & 0.6455 & 0.2886 \\ 0.8666 & 0.5000 & -1.5 & 0.5000 & 0.6455 & 0.2886 \\ 0 & 0.5000 & 0.5000 & -1.5 & 0.6455 & 1.1547 \\ 0 & 0.6455 & 0.6455 & 0.6455 & -4.5 & 0 \\ 0 & 0.2886 & 0.2886 & 1.1547 & 0 & 0 \end{bmatrix}. \quad (1)$$

In order not to lose the sparsity, we may as well think of how to get a simple low-dimensional representation (not requiring a good basis) without newly generating nonzero entries. In this paper, we study on such a representation (using a non-Hermitian matrix like

$$\begin{bmatrix} 1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2 & 0 & 0 \\ 0.5 & 0 & 2 & -1 & 1 & 0.5 \\ 0 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 6 & 0 & -3 \end{bmatrix} \quad (2)$$

that is sparse and consists of much simpler numbers than (1)) which can easily be obtained and used to calculate exact eigenvectors and eigenvalues more efficiently. Using (2) and orbit sizes (a vector of dimension 6), energies including the ground state energy of the 8-site Heisenberg spin-1/2 cube can exactly be calculated. We present the details about this approach herein.

To be specific, we show how to obtain a compressed representation of an irreducible Hamiltonian of the spin-1/2 Heisenberg antiferromagnet on the $L \times L$ lattice.⁶ The Heisenberg XXX ($J_x = J_y = J_z = J$) model (without an external magnetic field term, N_{spins} : number of all spin-sites) is defined as

$$H_{\text{Heisenberg}} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle ij \rangle} \sum_{\alpha \in \{x,y,z\}} \bigotimes_{k=1}^{N_{\text{spins}}} \left\{ (1 - \delta_{ik} - \delta_{jk}) I + (\delta_{ik} + \delta_{jk}) S^\alpha \right\} \quad (3)$$

$$\left(I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad S^x = \frac{1}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad S^y = \frac{1}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad S^z = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (\text{set } \hbar = 1) \right)$$

where δ_{ij} is the Kronecker delta ($\delta_{ij} = 1$ for $i = j$, otherwise $\delta_{ij} = 0$), and $\sum_{\langle ij \rangle}$ is the sum over nearest-neighbor sites i and j . In the case when $J_x = J_y$ (XXZ model), the relation $S^\pm = S^x \pm iS^y$ is used to re-express (3) as follows:

$$H_{\text{Heisenberg}} = J \sum_{\langle ij \rangle} \sum_{\alpha \in \{s_{ik}, s_{jk}, z\}} \bigotimes_{k=1}^{N_{\text{spins}}} \left\{ (1 - \delta_{ik} - \delta_{jk}) I + (\delta_{ik} + \delta_{jk}) S^\alpha \right\} \quad (4)$$

$$\left(\begin{array}{l} s_{lm} \text{ denoting } + \text{ if } l = m \\ s_{lm} \text{ denoting } - \text{ if } l \neq m \end{array}, \quad S^+ = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad S^- = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \right).$$

Note that when the number of all spins is even, the dimension of the irreducible block of the Hamiltonian (number of magnons constrained) is

$$\frac{N_{\text{spins}}!}{(N_{\text{spins}}/2)! (N_{\text{spins}}/2)!} = \frac{2^{N_{\text{spins}}} \Gamma(N_{\text{spins}}/2 + 1/2)}{\sqrt{\pi} \Gamma(N_{\text{spins}}/2 + 1)} \quad (5)$$

for the ground state computation. This exponential increase of the matrix dimension in proportion to the number of spin sites (“curse of dimensionality”³) practically limits $N_{\text{spins}} \lesssim 40$ in exact diagonalization studies.^{7,8} For the 36-site periodic lattices, the dimension of the minimal Hilbert space for the exact ground state computation is greater than 10^7 (10 million).^{9,10} The Hilbert space’s dimension for the 36-site non-periodic lattice (for the ground state computation) is approximately 10^9 with full symmetry group being considered. Meanwhile, tensor network (TN) variational methods¹¹ (data-sparse approximation³) have been studied to manage such lattices.^{12,13} The 36-site periodic kagomé lattice’s approximate ground state energy was computed using a TN method,¹³ which is 0.5% above the exact result by the Lanczos method.¹⁰ While matrix product state (MPS) has been proven a very powerful

tool for one-dimensional strongly correlated quantum lattice systems,¹⁴ TN methods generally have computational difficulties which arise from the amount and structure of the entanglement in quantum many-body states.¹¹

Notwithstanding these difficulties, the use of the compressed representation can effectively be used to calculate exact solutions to such large-scale spin lattice problems in that the compression is a simple process which does not calculate new matrix elements with no change of basis. After the compressed representation is obtained, a modified form of an eigensolver can be utilized. Without loss of data-sparsity, the ideas introduced in the following section permit us to effectively save hardware memory and computational time in real computation.

II. METHOD

Before introducing the algorithm providing the compressed representation of an irreducible Hamiltonian, we first define the representatives of the spin states. In addition, we briefly mention the relation between the representatives and the Hilbert space.

Let a $L \times L$ non-periodic lattice be on the x - y plane symmetrically about both the x -axis and the y -axis with the center of the lattice being at the origin $(0, 0)$. Consider the spin-1/2 Heisenberg XXZ antiferromagnet on this square lattice (Hamiltonian: H), the Hilbert space of which is $\mathcal{H} = \{|0\rangle, |1\rangle, \dots, |2^{L^2} - 1\rangle\}$ (\exists total 2^{L^2} spin arrangements). Note that the symmetry group of this lattice is Dih_4 (dihedral group of order 8), and so the group action

$$\phi : Dih_4 \times \mathcal{H} \rightarrow \mathcal{H}, \quad (6)$$

which transforms the coordinates of the spin sites on the square lattice, can be defined. For convenience, let us write

$$\phi(g, |k\rangle) = \phi_g |k\rangle \quad (7)$$

where $g \in Dih_4$ and $0 \leq k \leq 2^{L^2} - 1$. Also, let us define an index map $i_{\text{self}} : \mathcal{H} \rightarrow \mathbb{Z}^*$ (\mathbb{Z}^* : set of nonnegative integers) such that $i_{\text{self}}(|k\rangle) = k$ for $0 \leq k \leq 2^{L^2} - 1$. Then, we can define an index map $i_{\text{rep.}} : \mathbb{Z}^* \rightarrow \mathbb{Z}^*$ such that for $0 \leq k \leq 2^{L^2} - 1$,

$$i_{\text{rep.}}(k) = \text{Min} \left(\bigcup_{g \in Dih_4} \{i_{\text{self}}(\phi_g |k\rangle)\} \right), \quad (8)$$

which defines the representatives of the spin states.

Meanwhile, we denote the total spin in the z -direction by

$$S_{\text{tot.}}^z = \frac{L^2}{2} - M \quad (9)$$

where M is the number of magnons (spin flips). Then, we can express

$$\mathcal{H} = \bigoplus_{M=0}^{L^2} \mathcal{H}_M \quad (10)$$

where the Hamiltonian associated with \mathcal{H}_M is H_M (irreducible matrix), the dimension of which is written as

$$\dim(H_M) = \frac{L^2!}{M!(L^2 - M)!}. \quad (11)$$

Using the definition of i_{self} and $i_{\text{rep.}}$, \mathcal{H}_M can be expressed as

$$\mathcal{H}_M = \bigcup_{k \in i_{\text{rep.s}}(\mathcal{H}_M)} \bigcup_{g \in Dih_4} \{\phi_g |k\rangle\} \quad (12)$$

where

$$i_{\text{rep.s}}(\mathcal{H}_M) = \bigcup_{\psi \in \mathcal{H}_M} \{i_{\text{rep.}}(i_{\text{self}}(\psi))\}. \quad (13)$$

TABLE I. An algorithm for obtaining the compressed representation $(H_{M,\text{comp.}}, O_{\text{size}})$ for the spin-1/2 Heisenberg antiferromagnet on the $L \times L$ non-periodic lattice (Hamiltonian: H_M).

1.	Allocate a bit array R_{checker} of size $2^{N_{\text{spins}}}$ (dimension of H , $N_{\text{spins}} = L^2$) such that $R_{\text{checker}}[j] = 0$ for $1 \leq j \leq 2^{N_{\text{spins}}}$.
2.	For $1 \leq j \leq 2^{N_{\text{spins}}}$, set $R_{\text{checker}}[\text{irep.}(j)] = 1$ if the number of the spin flips of $ j\rangle$ is M .
3.	Take $k=0$. Then, for $1 \leq j \leq 2^{N_{\text{spins}}}$, if $R_{\text{checker}}[j] = 1$, $k++$ and $R_{\text{map}}(j) = k$ ($++$: increment operator). After this loop, take $N_{\text{orbits}} = k$
4.	For $1 \leq j \leq N_{\text{orbits}}$, we take $O_{\text{size}}[j] = \left \bigcup_{g \in \text{Dih}_4} \{i_{\text{self}}(\phi_g R_{\text{map}}^{-1}(j))\} \right $.
5.	For $1 \leq i \leq N_{\text{orbits}}$, obtain a set of indices $S_{\text{neighbor}}(i) = \bigcup_{\substack{1 \leq j \leq 2^{N_{\text{spins}}} \\ H_M[R_{\text{map}}^{-1}(i)][j] \neq 0}} \{j\}$.
6.	Let all the entries of $H_{M,\text{comp.}} \in \mathbb{R}^{N_{\text{orbits}} \times N_{\text{orbits}}}$ be zero. After that, for $1 \leq i \leq N_{\text{orbits}}$ and for $j \in S_{\text{neighbor}}(i)$, $H_{M,\text{comp.}}[i][R_{\text{map}}(\text{irep.}(j))] += H_M[R_{\text{map}}^{-1}(i)][j]$ ($+=$: addition assignment operator). (Note: The sparsity of H_M should be taken into account for computational efficiency.)
7.	Finally, we have the compressed representation $(H_{M,\text{comp.}}, O_{\text{size}})$ of H_M (Hamiltonian of the Heisenberg spin-1/2 antiferromagnet on the $L \times L$ non-periodic lattice with the number of magnons being M).

Based on the above, the algorithm in Table I provides a vector O_{size} and a matrix $H_{M,\text{comp.}}$ of dimension $|\text{irep.s}(\mathcal{H}_M)|$ with which exact eigenvalues of H_M are computed (“comp.” meaning compressed). Here, the vector O_{size} contains every orbit’s size (defined by the group action ϕ). Also, a submatrix of H_M and weighting numbers can construct $H_{M,\text{comp.}}$. We define the pair $(H_{M,\text{comp.}}, O_{\text{size}})$ as the compressed representation of H_M . Once we obtain $(H_{M,\text{comp.}}, O_{\text{size}})$, it is possible to obtain exact eigenvalues of H_M by computing a compressed vector of dimension $\dim(H_{M,\text{comp.}}) = N_{\text{orbits}}$ (orbit: vertex-orbit in graph theory). Note that even if the coupling constants J_x and J_z are changed, we can still make use of the previously obtained compressed representation since it is only necessary to multiply the diagonal and off-diagonal parts (nonzero elements) of H_M by some constants, respectively. For computational conveniences, it is possible to modify the algorithm and some mathematical representations. Instead of using $H_{M,\text{comp.}}$, for instance, it is possible to separately handle a submatrix of H_M and weighting numbers. They can be expressed bitwise since the weights cannot exceed the order of the symmetry group, so that an efficient data storage is possible.

Once the compressed representation $(H_{M,\text{comp.}}, O_{\text{size}})$ is obtained, we can calculate eigenvalues with it. For example, in order to obtain the ground state energy, we can utilize the variant of the power iteration as follows. First, take a random vector $\mathbf{u}_1 \in \mathbb{R}^{N_{\text{orbits}}}$ and a large enough value $\lambda' \in \mathbb{R}^+$ (to get the lowest energy and to avoid a convergence problem). For $1 \leq i \leq N_{\text{orbits}}$, do $H_{M,\text{comp.}}[i][i] -= \lambda'$ ($-=$: subtraction assignment operator). For $\mathbf{v} \in \mathbb{R}^{N_{\text{orbits}}}$, $\mathbf{u}_k \in \mathbb{R}^{N_{\text{orbits}}}$, and $k \in \mathbb{N}$, we define

$$\|\mathbf{u}_k\|_{\text{comp.}} = \sqrt{\sum_{l=1}^{N_{\text{orbits}}} O_{\text{size}}[l] \cdot (\mathbf{u}_k)_l \cdot (\mathbf{u}_k)_l}, \quad (14)$$

$$\tilde{\mathbf{u}}_k = \frac{1}{\|\mathbf{u}_k\|_{\text{comp.}}} \mathbf{u}_k \text{ and } \mathbf{u}_{k+1} = H_{M,\text{comp.}} \tilde{\mathbf{u}}_k. \quad (15)$$

Then, as k increases, $\lambda + \lambda'$ converges to the lowest energy of H_M where

$$\lambda = \sum_{l=1}^{N_{\text{orbits}}} O_{\text{size}}[l] \cdot (\tilde{\mathbf{u}}_k)_l \cdot (H_{M,\text{comp.}} \tilde{\mathbf{u}}_k)_l. \quad (16)$$

III. RESULTS

Here, we demonstrate the computational performance of the method in Section II applied to the spin-1/2 Heisenberg antiferromagnet on the $L \times L$ non-periodic lattice (expressed by the irreducible matrices H_M in Section II ($\dim(H_M) = n_M$)). For $2 \leq L \leq 6$, we present the calculated lowest energies

TABLE II. Computed energies (exact) in unit of J . The 1st excited energy is obtained using the reorthonormalization after the lowest energy computation.

L	lowest energy	1st excited energy
2	-2.00000000	-1.00000000
3	-4.74932726	-3.75865635
4	-9.18920706	-7.79090797
5	-14.69614643	-14.13765455
6	-21.72678604	-20.88907857

(exact) in Table II using the method in Section II (data-sparsity considered in computation). In the following Tables, the advantages coming from the use of this representation are demonstrated. When the power iteration is used, an $O(n_M)$ calculation is required to obtain an eigenvalue due to the matrix's sparsity. Meanwhile, if we use the variant of the power iteration with the compressed representation here, only an $O(kn_M)$ calculation is required where k decreases toward 1/8 as L increases. It reflects the fact that the sparsity of the original matrix is well retained in this representation.

A. Dimension reduction

The use of the compressed representation of the irreducible matrix H_M (Refer to Section II.) makes it possible to save both computational resources and computational time in real computation. Although any change of basis is not applied here, the additional dimension reduction is easily achieved as shown in Table III. Notice that $\frac{\dim(H_M)}{\dim(H_{M,\text{comp.}})}$ converges to 8 (order of the symmetry group of square) as L increases.

B. Data size reduction

The dimension reduction in Table III directly results in the reduction of the size of the data constructed from the irreducible Hamiltonian H_M . Here, data-sparsity was considered when the data of H_M and $(H_{M,\text{comp.}}, O_{\text{size}})$ were generated, the sizes of which (in bytes) are shown in Table IV. It is remarkable that the ratio in Table IV also converges to 8 as L increases, implying that $(H_{M,\text{comp.}}, O_{\text{size}})$ well retains the data-sparsity of H_M .

C. Computational time reduction

The data size reduction naturally gives rise to the computational time reduction. In comparison to obtaining H_M and using the power iteration, the method in Section II diminishes the computational

TABLE III. Dimension reduction.

L	$\dim(H)$	$\dim(H_M)$	$\dim(H_{M,\text{comp.}})$	$\frac{\dim(H)}{\dim(H_M)}$	$\frac{\dim(H_M)}{\dim(H_{M,\text{comp.}})}$
2	16	6	2	2.667	3.000
3	512	126	23	4.064	5.478
4	65536	12870	1674	5.092	7.688
5	33554432	5200300	652048	6.452	7.975
6	68719476736	9075135300	1134460910	7.572	8.000

TABLE IV. Data size in bytes.

L	H_M	$(H_{M,\text{comp.}}, O_{\text{size}})$	Ratio
2	1.340×10^2	3.400×10^1	3.941
3	5.334×10^3	7.540×10^2	7.074
4	9.395×10^5	1.190×10^5	7.893
5	5.928×10^8	7.413×10^7	7.997
6	1.491×10^{12}	1.864×10^{11}	8.000

TABLE V. Computational time in seconds (GS: the ground state) using a single core of Intel(R) Xeon(R) CPU E5-2620 v2 @ 2.10GHz. (*: approximate estimation based on parallel computation)

L	GS from H_M	GS from $(H_{M,\text{comp.}}, O_{\text{size}})$	Ratio
2	3.414×10^{-6}	1.353×10^{-6}	2.523
3	9.493×10^{-5}	2.111×10^{-5}	4.497
4	2.027×10^{-2}	3.231×10^{-3}	6.274
5	1.011×10^2	1.361×10^1	7.428
6	No data	$*1 \times 10^5$	None

time for obtaining eigenvalues as described in Table V. As L increases, the ratio in Table V tends to vary in accordance with the ratio variances in Tables III and IV. Here, a C++ program and a single core of Intel(R) Xeon(R) CPU E5-2620 v2 @ 2.10GHz were used for benchmarking. Compared to the computation time (without I/O) of the ground state using $(H_{M,\text{comp.}}, O_{\text{size}})$ (with the sparsity of H_M being considered), it takes a similar length of time to obtain $(H_{M,\text{comp.}}, O_{\text{size}})$ even when `std::map` and data I/O process (trade-off between speed and memory) are used. In the same condition (including optimization flags), the Lanczos routine^{15,16} in SPINPACK¹⁷ spent about 50 seconds calculating the ground state energy for $L = 5$ from a low-rank block matrix (full symmetry group considered). Practically, the method in Section II could be a good alternative when performing this kind of calculation. The development of a variant of the Lanczos method using $(H_{M,\text{comp.}}, O_{\text{size}})$ may possibly improve the speed of computation even more.

IV. DISCUSSION AND CONCLUDING REMARKS

In this paper, it has been shown that we can make use of a compressed representation of an irreducible Hamiltonian matrix. We have dealt with the spin-1/2 Heisenberg antiferromagnet on a square lattice (non-periodic) as a practical application. It directly indicates that such a low-dimensional representation can be utilized in other Heisenberg models as well as the t - J model and the Hubbard model in solid state physics. The use of the compressed representation allows us to save both computational resources and computational time since not only is it sparse as original matrix, we do not need to compute a new basis and new matrix elements to obtain low-rank matrices. At this point, we may cast the following question: ‘‘How can we mathematically generalize this approach in various aspects?’’ Algebraic graph theory is possibly a good tool for the remaining mathematical works.

From a graph theoretical point of view, an irreducible matrix $W \in \mathbb{R}^{n \times n}$ (the entry in row i , column j : w_{ij}) is irreducible if and only if its associated graph $\mathcal{G} = (V, A_W)$ is strongly connected² where $V(\mathcal{G}) = \{v_1, \dots, v_n\}$ is the set of all vertices of \mathcal{G} , and $A_W(\mathcal{G}) = \{\{v_i, v_j\}, w_{ij} : 1 \leq i \leq n, 1 \leq j \leq n, w_{ij} \neq 0\}$ is the set of all weighted arcs of \mathcal{G} . Meanwhile, we denote by $\text{Aut}(\mathcal{G})$ the set of every automorphism $\phi : \mathcal{G} \rightarrow \mathcal{G}$ defined by $\varphi_\phi : V(\mathcal{G}) \rightarrow V(\mathcal{G})$ with $\{\{v_i, v_j\}, w_{ij}\} \in A_W(\mathcal{G})$ if and only if $\{\{\varphi_\phi(v_i), \varphi_\phi(v_j)\}, w_{ij}\} \in A_W(\mathcal{G})$ for all $i, j \in \{1, \dots, n\}$.¹⁸ Here, $\text{Aut}(\mathcal{G})$ always forms a permutation group by the following facts: 1) the composition of two automorphisms of \mathcal{G} is an automorphism of \mathcal{G} , and 2) the inverse of an automorphism of \mathcal{G} is also an automorphism.¹⁹ If \mathcal{G} is asymmetric, $\text{Aut}(\mathcal{G})$ is the identity group.²⁰ Otherwise, there exist one or more nontrivial vertex orbits of \mathcal{G} since $|\text{Aut}(\mathcal{G})| > 1$. From this viewpoint, it is possible to say that the compressed representation of an irreducible matrix can be defined unless its associated graph is asymmetric. Based on graph measures and metrics, we are able to define compression policies (providing exact/approximate solutions) for general purposes and make use of an automated policy selector aided by a machine learning technique. In this regard, we suggest that the ideas presented here should be investigated from the graph theoretical point of view for further researches.

As is applied in the power iteration, similarly, it is worth relating the compressed representation of an irreducible matrix to the other eigensolvers carrying out, e.g. subspace iteration, computing all eigenpairs, etc. Additionally, defining new operations based on the compressed representation of an irreducible matrix would possibly lead to the improvements and the developments of various computational methods. At the same time, further rigorous mathematical works are also necessary regarding this idea. Applied to existing methods, their computational costs can also be lowered if there

is an utilizable symmetric structure. We anticipate that this simple point of view on the “reducibility” of irreducible matrices could shed light on a pathway to substantially resolving computational difficulties in various fields using matrix computations and discovering other useful methodologies.

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