Exact-diagonalization method for correlated-electron models

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We present a method to compute eigenstates and eigenvalues of strongly correlated models on clusters. The calculation is performed applying the SU(2) symmetry, which allows a considerable reduction of the dimension of Hilbert space of the system. We illustrate the method classifying the states of the four-sites Hubbard model on a chain. This classification has been made using also the translational symmetry and the $\widetilde{\mathrm{SU}}(2)$ pseudospin symmetry. [S0163-1829(96)09241-7]

I. INTRODUCTION

The theoretical description of electronic correlations in the intermediate and strong coupling regimes is a long standing problem. Following the discovery of heavy-fermion compounds, and more recently, of the high-temperature superconductors, these problems have attracted renewed attention.[1]

Unfortunately, for models used to describe the above mentioned systems, very few exact results are known, a noticeable exception being the one-dimensional situation where in many cases the exact solution is available.[2] In more than one dimension many important physical questions remain unsolved, despite the great number of different theoretical approaches that have been applied. In absence of exact results, a reliable way to describe the properties of strongly correlated models is to resort to numerical techniques. These techniques have proved to be the only practical tool to study finite size systems, also due to the rapid increase in computer performances.[3]

The two techniques by far most intensively used are Lanczos[4] and Monte Carlo (MC) methods,[5] but regretfully these methods have also limitations. The MC approach allows to handle sufficiently large systems so that the results are physically of great interest in trying to predict the behavior of the system in the thermodynamic limit. However, because of the so called sign problem, which enormously enhances the statistical uncertainties of simulations, the maximum size of the lattice to be described is confined to a few tens of sites. In this case the exact diagonalizations become competitive being in general more precise.

Lanczos calculations give essentially exact results for ground-state, low lying eigenvectors and quantities such as single particle excitation spectra.[4] In spite of these advantages, memory limitations impose severe restrictions on the size of clusters that can be studied within this method. Usually the basis set of vectors employed in the diagonalization procedure grows exponentially with the system size. This problem can be considerably alleviated using the symmetries of the Hamiltonian that reduce the matrix Hamiltonian to a block form. The most obvious symmetry is the U(1) symmetry that is usually conserved at least for fermionic problems. The third component of total spin operator **S** may also be a good quantum number and, for translational invariant Hamiltonians, the total momentum **P** of the system is conserved as well. Upon the implementation of these symmetries, the linear size of the blocks to be diagonalized is strongly reduced. For instance, for a 4×4 Hubbard model, at half filling, $S_z=0$ and zero momentum the largest block is about 1.35×10^6.[6]

It is then obvious that the use of symmetries is crucial in performing Lanczos calculations on large clusters. In many cases the symmetries of the problem are not exhausted by the ones cited above. Several Hamiltonians exhibit other symmetries such as spin inversion, rotations about a given site, reflections with respect to lattice axes, the $\widetilde{\mathrm{SU}}(2)$ pseudospin symmetry[7] and so on. Among them, it is worth stressing that the SU(2) spin symmetry until now has not been applied in the diagonalization procedures.

Here we present a technique to calculate the eigenvectors and eigenvalues for strongly correlated models on moderately large clusters based on the application of SU(2). To illustrate our method, we consider as an example the one-dimensional Hubbard model with periodic boundary conditions with an even number of sites.[7]

The paper is organized as follows: the method to compute eigenstates and eigenvalues of the Hubbard model is given in Sec. II, while in Sec. III is presented, as application of the method previously introduced, the calculation of the full spectrum of the Hubbard model on four-site ring together with a complete characterization of the ground state in the half filled case: finally Sec. IV is devoted to the conclusions.

II. THE METHOD

It is well known that on a bipartite lattice the Hubbard Hamiltonian

$$H=\sum_{ij,\sigma}(t_{ij}-\mu\delta_{ij})c^{\dagger}_{i\sigma}c_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow} \tag{1}$$

has two independent SU(2) symmetries in spin and pseudospin space, which involve the spin and the charge degrees of freedom, respectively. The first one, which reflects the invariance of H under spin rotation, is the ordinary SU(2) symmetry in spin space, characterized by the generators

$$S^z=\frac{1}{2}\sum_i (c^\dagger_{i\uparrow}c_{i\uparrow}-c^\dagger_{i\downarrow}c_{i\downarrow}), \tag{2}$$

$$S^+=\sum_i c^\dagger_{i\uparrow}c_{i\downarrow}, \tag{3}$$

$$S^-=\sum_i c^\dagger_{i\downarrow}c_{i\uparrow}. \tag{4}$$

The second $\widetilde{\mathrm{SU}}(2)$ symmetry can be generated by a particle-hole transformation involving only one kind of spin, say $c_{i\downarrow}\rightarrow(-1)^i c^\dagger_{i\downarrow}$, which maps at half filling the repulsive-U Hubbard model to an attractive-U one. The fact that this latter model also has rotational symmetry in its spin space implies that the Hamiltonian (1) is invariant under the action of a second group, that we denote by $\widetilde{\mathrm{SU}}(2)$, whose generators are

$$J^z=\frac{1}{2}\sum_i (c^\dagger_{i\uparrow}c_{i\uparrow}+c^\dagger_{i\downarrow}c_{i\downarrow}-1), \tag{5}$$

$$J^+=\sum_i (-1)^i c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}, \tag{6}$$

$$J^-=\sum_i (-1)^i c_{i\downarrow}c_{i\uparrow}. \tag{7}$$

The connection between the $\widetilde{\mathrm{SU}}(2)$ symmetry and the charge degrees of freedom is evident from the fact J_z is nothing but the charge operator. The commutation relations

$$[H,J^\pm]=\pm(U-2\mu)J^\pm$$

imply that away from half filling the global invariance under the $\widetilde{\mathrm{SU}}(2)$ group is lost. However, being $[H,J^2]=[H,J_z]=0$ for any value of $U-2\mu$, the characterization of the eigenstates of H in terms of the eigenvalues of J^2 and J_z is always possible. Moreover, the fact that $J^\pm$ are eigenoperators of H allows us to obtain the eigenenergies within a multiplet with given J from the relation

$$H|J,J-n\rangle=H(J^-)^n|J,J\rangle=(E_{JJ}+n(U-2\mu))|J,J-n\rangle,$$

where $0\leqslant n\leqslant 2J$, and E_{JJ} is the energy of the highest pseudospin state.

When cyclic boundary conditions are assumed, one can further reduce the size of the Hamiltonian matrix blocks specifying the eigenstates of H in terms of the eigenvalues of the translation operator T. It is worth noting that, in the generation of a J-multiplet from the highest J_z state, the application of J^- always changes the sign of the corresponding eigenvalue of T. Indeed, from the anticommutation relations $[T,J^\pm]_+=0$ one has that, if $T|\alpha\rangle=\lambda|\alpha\rangle$, then $T[(J^-)^n|\alpha\rangle]=(-1)^n\lambda[(J^-)^n|\alpha\rangle]$.

For each site i the four states $|0\rangle_i,|\uparrow\rangle_i,|\downarrow\rangle_i$, and $|\uparrow\downarrow\rangle_i$ form a basis of the local Hilbert space. Alternatively, we can classify the states of the Hilbert space giving the occupation of each site, so that $|2\rangle_i$ denotes a doubly-occupied $|1\rangle$, a singly-occupied, and $|0\rangle$, an unoccupied i site. The doubly occupied and the empty site states are eigenstates of S^2 and S_z with zero eigenvalue. This amounts to say that they do not affect the total spin of the configuration, so that to determine the eigenvectors of S^2 for a given filling, we are left with the composition of one-half spins on singly occupied sites. Therefore for a model defined on N sites, the only problem is the composition of N spins at most.

Let us apply the $\widetilde{\mathrm{SU}}(2)$ symmetry. First of all, we notice that $|2\rangle_i$ and $(-)^i|0\rangle_i$ are eigenstates of J_{zi} with eigenvalues $\frac{1}{2}$ and $-\frac{1}{2}$, respectively, and $|1\rangle_i$ is eigenstate of J_i^2 and J_{zi} with zero eigenvalue. Thus the states representing the singly occupied sites do not affect the total pseudospin of a given configuration and we have to add only the pseudospin of states having double and zero occupancy. This means that the same technique previously introduced for the SU(2) symmetry can be applied to the $\widetilde{\mathrm{SU}}(2)$ pseudospin symmetry.

Finally we apply the translational symmetry making use of the notation presented here. Let us define the translation operator T through the relation

$$T[|\cdot\rangle_1|\cdot\rangle_2\cdots|\cdot\rangle_N]=|\cdot\rangle_2|\cdot\rangle_3\cdots|\cdot\rangle_1. \tag{8}$$

This operator does not change the type of configuration in the sense that it does not affect the number of doubly-occupied, singly-occupied, and empty sites. Besides, it is easy to see that holds the following relation:

$$T^k|\alpha\rangle=\pm|\alpha\rangle, \tag{9}$$

where $|\alpha\rangle$ is a generic state and k is an integer such that $k=N$ or $k=N/l$ with l integer ($\neq N$). From this relation, we see that $T^k=\pm I$, I being the identity operator, and thus we can write k eigenstates of T in the following way:

$$|\phi_{\lambda_{m\pm}}\rangle=\frac{1}{\sqrt{k}}\sum_{j=0}^{k-1} e^{(it_{m\pm}j)}T^j|\alpha\rangle, \tag{10}$$

where $t_{m+}=2m\pi/k$, $t_{m^-}=2m\pi/k+\pi/k$, $\lambda_{m\pm}=\exp(-it_{m\pm})$, and $m=0.1,\ldots,k-1$. We notice that the eigenvalues of T are given by $\lambda_{m\pm}=\exp(-it_{m\pm})$ with $m=0.1,\ldots,k-1$. The state $|\alpha\rangle$ which gives rise to the eigenstate of T with eigenvalue $\lambda_{m\pm}$ is defined as the generator of that eigenstate.

It is worth noticing that the construction of $\{|\phi\rangle\}$ states is not restricted to one-dimensional cases but it can be immediately extended to other spatial symmetries in more than one dimension.

III. APPLICATION OF THE METHOD

Let us now illustrate our method by considering the Hubbard model on a four-site ring. According to the technique introduced in Sec. II at half filling the possible configurations are

$$\text{(a)}\quad |2\rangle_i|2\rangle_j|0\rangle_k|0\rangle_l, \tag{11}$$

$$\text{(b)}\quad |2\rangle_i|1\rangle_j|1\rangle_k|0\rangle_l, \tag{12}$$

$$\text{(c)}\quad |1\rangle_1|1\rangle_2|1\rangle_3|1\rangle_4, \tag{13}$$

where the subscript denotes the lattice site $(i,j,k,l=1,2,3,4)$.

In case (a) we have $S^2|2\rangle_i\,|2\rangle_j\,|0\rangle_k\,|0\rangle_l=0$ for any i,j,k,l. In case (b) adding two spins $\frac{1}{2}$ we trivially obtain a triplet and a spin singlet state. Permutating the lattice indices we can

TABLE I. Classification of the basis states of the four-site Hubbard model in terms of the eigenvalues of the spin, the pseudospin, and the translation operator.

Generators	T representation	S	J	λ	Number of states
	T_1^*	2	0	-1	5
$T_{13}\oplus T_{24}$	T_1	1	0	1	3
	T_1^*	0	0	-1	1
$T_{13}\oplus S_{24}$	T_2^*	1	0	$\pm i$	6
$S_{13}\oplus S_{24}$	T_1	0	0	1	1
	T_1	0	2	1	5
$t_{13}\oplus t_{24}$	T_1^*	0	1	-1	3
	T_1	0	0	1	1
$t_{13}\oplus s_{24}$	T_2^*	0	1	$\pm i$	6
$s_{13}\oplus s_{24}$	T_1^*	0	0	-1	1
$T_{12}\oplus t_{34}$	T_4	1	1	$\pm 1,\pm i$	36
$T_{13}\oplus t_{24}$	T_2^*	1	1	$\pm i$	18
$T_{12}\oplus s_{34}$	T_4	1	0	$\pm 1,\pm i$	12
$T_{13}\oplus s_{24}$	T_2	1	0	± 1	6
$s_{12}\oplus t_{34}$	T_4	0	1	$\pm 1,\pm i$	12
$S_{13}\oplus t_{24}$	T_2	0	1	± 1	6
$S_{12}\oplus s_{34}$	T_4	0	0	$\pm 1,\pm i$	4
$S_{13}\oplus s_{24}$	T_2^*	0	0	$\pm i$	2
$T_{12}\oplus D_3\oplus d_4$	T_4	$\frac{3}{2}$	$\frac{1}{2}$	$\pm 1,\pm i$	32
	T_4	$\frac{1}{2}$	$\frac{1}{2}$	$\pm 1,\pm i$	16
$S_{12}\oplus D_3\oplus d_4$	T_4	$\frac{1}{2}$	$\frac{1}{2}$	$\pm 1,\pm i$	16
$t_{12}\oplus d_3\oplus D_4$	T_4	$\frac{1}{2}$	$\frac{3}{2}$	$\pm 1,\pm i$	32
	T_4	$\frac{1}{2}$	$\frac{1}{2}$	$\pm 1,\pm i$	16
$s_{12}\oplus d_3\oplus D_4$	T_4	$\frac{1}{2}$	$\frac{1}{2}$	$\pm 1,\pm i$	16

write down all the eigenstates of S^2 and S_z for these configurations. Finally in case (c) we have to sum up four spins which gives one spin $S=2$ state, three triplets and two singlets.

In order to apply the $\widetilde{\mathrm{SU}}(2)$ pseudospin symmetry, we notice that the role of singly-occupied sites $|1\rangle$ with respect to the SU(2) symmetry, for $\widetilde{\mathrm{SU}}(2)$ symmetry, is played by states having double and zero occupancy.

Let us finally apply the translation symmetry. To be specific we discuss the application of T on states having two double occupancy [(a) configurations]. Applying T^n to $|2\rangle_1\,|2\rangle_2\,|0\rangle_3\,|0\rangle_4$ we obtain $|2\rangle_2\,|2\rangle_3\,|0\rangle_4\,|0\rangle_1$, $|2\rangle_3\,|2\rangle_4\,|0\rangle_1\,|0\rangle_2$, $|2\rangle_4\,|2\rangle_1\,|0\rangle_2\,|0\rangle_3$, and $|2\rangle_1\,|2\rangle_2\,|0\rangle_3\,|0\rangle_4$, for $n=1,2,3,4$, respectively. This means that $T^4=I$ and consequently its eigenvalues λ_i are ± 1, $\pm i$. Besides, in this subspace T has the following matrix representation:

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Not all the states of (a) type are connected by T: indeed the state $|2\rangle_1\,|0\rangle_2\,|2\rangle_3\,|0\rangle_4$ is related to $|2\rangle_2\,|0\rangle_3\,|2\rangle_4\,|0\rangle_1$. For these states $T^2=I$ and $\lambda_i=\pm 1$. The same consideration can be made for (b) and (c) configurations and for states having $\widetilde{\mathrm{SU}}(2)$ symmetry, so that we can group the states in blocks of dimension 4 or 2. According to the definition given in Sec. II, the states $|2\rangle_1\,|2\rangle_2\,|0\rangle_3\,|0\rangle_4$ and $|2\rangle_1\,|0\rangle_2\,|2\rangle_3\,|0\rangle_4$ are the generators of vector basis states having two doubly occupied sites.

The diagonalization of the four-site Hamiltonian in terms of S^2 and S_z leads to matrix blocks whose maximum dimension is 20×20 (reached at half filling for $S=S_z=0$). The application of the $\widetilde{\mathrm{SU}}(2)$ symmetry reduces to 10×10 the size of the largest block, which is further split into two blocks of dimension 3×3 and 2 blocks of dimension 2×2 after the application of the translational invariance of H. The whole set of the Hamiltonian matrix blocks, labeled by the eigenvalues of S, J, J_z, and T, is reported for the half-filled case in the Appendix, having assumed $t_{ij}=-t(t>0)$ on nearest-neighbor sites, and $t_{ij}=0$ otherwise. It is worth noticing that a different scheme for diagonalizing the four-site Hubbard model has also been developed by Villet and Steeb,[8] taking into account the spin reversal and the C_{4v} symmetry of the Hamiltonian. With this kind of choice, however, the reduction of the matrix block size is not as effective as it is in our case. In half filling, for instance, one is left with 7×7 matrix blocks, while in our approach the highest matrix size is 3×3. This is, of course, a significant difference, which becomes more and more relevant as larger clusters are considered.

All the eigenstates can be deduced from the Table I, where T, D, S (t, d, s) denote the triplet, doublet, and singlet for S^2 (J^2), respectively: the lower indices refer to the lattice sites and indicates the composition of spins or pseu-

dospin states. We notice that the configurations in the first column of the table are the simultaneous eigenstates of S^2 and J^2 and they are also the generators of basis vectors of irreducible representations of T; T_i is associated with the transformation $(T)^i=I$ on the corresponding generator states and $(T^*)^i=-I$.

For example to the generator $T_{13}\oplus s_{24}$ corresponds the (highest spin) state

$$|\alpha\rangle=|\uparrow\rangle_1|\uparrow\rangle_3\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle_2|0\rangle_4+|0\rangle_2|\uparrow\downarrow\rangle_4),$$

where $|\uparrow\rangle_1|\uparrow\rangle_3$ is the highest spin state of the triplet T_{13} and $(1/\sqrt{2})(|\uparrow\downarrow\rangle_2|0\rangle_4+|0\rangle_2|\uparrow\downarrow\rangle_4)$ is the s_{24} pseudospin singlet.

Applying the translation operator T to $|\alpha\rangle$ we obtain

$$T^2|\alpha\rangle=|\alpha\rangle.$$

that implies $\lambda_i=\pm1$. Keeping in mind that T_{13} denotes a spin triplet we have, for any λ_i, three different states corresponding to $S_z=\pm1,0$, so that $T_{13}\oplus s_{24}$ generates six states.

As previously mentioned, even though the exact solution of the Hubbard model has only been given in the one-dimensional case, some exact results in arbitrary dimension, concerning in particular the ground-state properties, are nonetheless available. In the following, we are going to give a complete characterization of the ground state of the four-site Hubbard model in terms of the above mentioned conserved quantities, with a special attention to the predictions of Lieb theorem.[9]

Lieb positive-U theorem states that if the repulsive Hubbard model at half filling is defined on a connected and bipartite lattice with an even number of sites, the ground state is unique [except for the $(2S+1)$ degeneracy] and has spin $S=|N_A-N_B|/2$, where N_A and N_B are the numbers of sites in the two sublattices A and B. We have verified in the four-site problem that for any positive U the theorem is satisfied. In agreement with the above theorem, it is found that for any value of the on-site repulsion the system is always in a ground state with $S=0$. Moreover, we have found that the eigenvalue of the pseudospin operator for the ground state is $J=0$ confirming the lemma by Shen and Qiu[10] that states that the ground state must be a pseudospin singlet, if the same assumptions of Lieb positive-U theorem are made. The set of all the eigenstates with $S=0$ and $J=0$ can be further split in subsets associated with the four possible eigenvalues $\lambda=1$, -1, i, $-i$ of the translation operator. The states belonging to the two subspaces associated with $\lambda=\pm i$ are of course degenerate in energy. The curves in Fig. 1 report the dependence on U of the ground-state energies in each of the above mentioned subspaces with $S=J=0$. Being associated with the eigenvalue $\lambda=-1$ of T, the ground state is found to be nondegenerate for any finite value of U, again in agreement with Lieb theorem.

IV. CONCLUSIONS

The technique introduced here can be easily applied to other one-band models such as the extended Hubbard, t-J, Heisenberg as well as to two-band models like p-d, Anderson, and so on. In these latter cases we define the possible configurations dividing the occupation of each site between the two type of electrons. In this way we have to double the number of configurations with respect to the number of sites. This implies that the Hilbert space for two-band N-sites models has the same dimension of $2N$-sites one-band models.

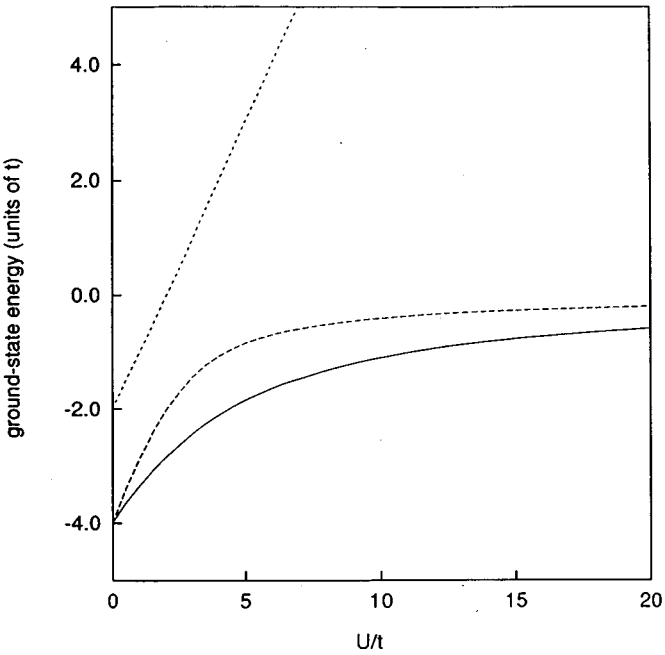

FIG. 1. Dependence on U of the ground-state energy in the subspaces with $S=0$, $J=0$, and $\lambda=-1$ (solid line), $\lambda=1$ (long-dashed line), and $\lambda=i$ (short-dashed line).

To conclude, in this paper we have presented a method to compute the eigenvalues and the eigenvectors for strongly correlated models on clusters. We have demonstrated the efficiency of the method classifying all the eigenstates of the four-sites Hubbard model. We believe that such an approach is quite general and might be useful in problems where the huge dimensions of the Hilbert space do not allow a straightforward implementation of standard algorithms. The knowledge of all the vectors of the Hilbert space overcomes the disadvantage of Lanczos method giving the opportunity to study also thermodynamical properties; on the other hand with respect to MC, where some restrictions are imposed to the range of parameters in order to avoid the sign problems, our technique does not depend on the parameters of the model and on the temperature. In future papers we will apply this method to some models for strongly correlated-electron systems, discussing thermodynamical as well as dynamical properties of the model.

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APPENDIX

We list here the whole set of blocks in which the Hamiltonian matrix is split in half filling, when the symmetries

under spin rotation, pseudospin rotation, and lattice translation are implemented. We use the notation $H_{S,J,\lambda}$ to denote the matrix representation of the Hamiltonian in the subspace with eigenvalues S,J,λ and with $J_z=0$ (which enforces the half-filling condition) and with the highest possible values of the spin component ($S_z=S$). It is easily verified that $H_{S,J,-i}=(H_{S,J,i})^*$, which implies that in these subspaces the corresponding eigenergies are doubly degenerate. The matrix blocks are

$$H_{0,0,1}=\begin{pmatrix} 2U & 0 & \sqrt{12}t \\ 0 & 0 & -2t \\ \sqrt{12}t & -2t & U \end{pmatrix},$$

$$H_{0,0,-1}=\begin{pmatrix} 0 & 0 & -\sqrt{12}t \\ 0 & 2U & 2t \\ -\sqrt{12}t & 2t & U \end{pmatrix},$$

$$H_{0,0,i}=\begin{pmatrix} U & \sqrt{2}(1+i)t \\ \sqrt{2}(1-i)t & U \end{pmatrix},$$

$$H_{0,1,1}=\begin{pmatrix} 2U & 0 & -\sqrt{8}t \\ 0 & U & \sqrt{8}t \\ -\sqrt{8}t & \sqrt{8}t & U \end{pmatrix},$$

$$H_{0,1,-1}=\begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix},$$

$$H_{0,1,i}=\begin{pmatrix} 2U & \sqrt{2}(1+i)t \\ \sqrt{2}(1-i)t & U \end{pmatrix},$$

$$H_{0,2,1}=(2U),$$

$$H_{1,0,1}=\begin{pmatrix} 0 & -\sqrt{8}t & 0 \\ -\sqrt{8}t & U & -\sqrt{8}t \\ 0 & -\sqrt{8}t & U \end{pmatrix},$$

$$H_{1,0,-1}=\begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix},$$

$$H_{1,0,i}=\begin{pmatrix} U & -\sqrt{2}(1-i)t \\ -\sqrt{2}(1+i)t & 0 \end{pmatrix},$$

$$H_{1,1,1}=H_{1,1,-1}=(U),$$

$$H_{1,1,i}=\begin{pmatrix} U & -\sqrt{2}(1-i)t \\ -\sqrt{2}(1+i)t & U \end{pmatrix},$$

$$H_{2,0,-1}=(0).$$

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