Schrieffer-Wolff Transformation on IBM Quantum Computer

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Schrieffer-Wolff transformation (SWT) has been extensively used in quantum many-body physics to calculate the low energy effective Hamiltonian. It provides a perturbative method to comprehend the renormalization effects of strong correlations in the quantum many-body models. The generator for Schrieffer-Wolff transformation is calculated usually by heuristic methods. Recently, a systematic and elegant method for the calculation of this extremely significant transformation has been reported [1]. Given the huge significance of SWT for many areas including quantum condensed matter physics, quantum optics and quantum cavity electrodynamics, it is imperative to develop quantum algorithm for carrying out SWT on quantum computer. In this paper, we put forward this quantum algorithm and demonstrate it for single impurity Anderson model (SIAM), thereby arriving at Kondo model as effective Hamiltonian. We implement our quantum algorithm in QisKit and carry out SWT for SIAM on IBM Quantum computers. To the best of our knowledge, this work is the first of its kind to obtain Kondo model from Anderson impurity model using a quantum algorithm.

1 Introduction

Comprehending and controlling quantum many-body systems is of immense importance in modern theoretical, computational and experimental physics [2, 3, 4]. As the Hilbert space grows exponentially, it is challenging to do exact analytical calculations with the increase in system size. In majority of applications, details about the low-energy features are enough, hence the description of the low-energy effective Hamiltonian ($H_{eff}$) has got a significant role in many-body physics [5].

Schrieffer-Wolff transformation (SWT) was initially proposed in [6] to connect Anderson impurity model with Kondo model in the strong coupling regime. Since then this unitary transformation has been employed excessively in condensed matter physics. In [7] recent review on SW transformation has been reported. There a mathematically rigorous description of the transformation has been presented. SWT can be regarded as a degenerate perturbation theory. For example, due to SWT we can deduce that the Heisenberg model in the strong coupling regime is effectively equivalent to the Fermi-Hubbard model [8, 9], where it becomes difficult to use approaches from perturbation theory [10]. Having being used and developed for myriad quantum problems [11, 12, 13, 14, 15, 42, 17, 18, 19, 20, 21, 22, 23, 24, 25], SWT has been christened by various names across different
fields: In semiconductor physics known as k.p method [26], in electron-phonon interaction called as Frohlich transformation [27] and in relativistic quantum mechanics named as Foldy-Wouthuysen transformation [28].

SWT transformation is exploited to calculate the effective Hamiltonians of the models for strongly correlated electron systems as well as various other quantum many-body systems. It can be interpreted as single shot renormalization process that projects out the high energy excitations. This then leads to the low energy effective Hamiltonians that have the signatures of the projected out high energy excitations manifested as renormalized coupling constants. Although SWT is having perturbative nature but it offers a technique that provides physical insights and intuitions regarding the quantum many-body systems in the strong coupling regime. One prototypical illustration is the derivation of the Kondo model as an effective Hamiltonian of the Anderson impurity model. Later, it was affirmed that Kondo model leads to the strong coupling fixed point of Anderson impurity model by using numerical renormalization group calculation. Moreover, one of its important aspects is the unitarity unlike some projective methods used for calculations of the effective Hamiltonians. SWT as a unitary transformation cuts the clutter of the off-diagonal terms up to the first order and thus turns out to be a way to diagonalization.

Recently, quantum computation has attracted ample attention. It has been shown that quantum computers are able in tackling problems that are intractable for classical computers [29, 30]. So it naturally becomes highly desirable to find an algorithm for this transformation that can be implemented on a quantum computer. In this paper, we for the first time propose a full quantum algorithm for a quantum computer to realize SWT.

The plan of the paper is as follows. In the next section brief introduction to SWT and review of relevant different approaches and interpretations is given. In section 3 a systematic method for SWT is discussed. In section 4, the quantum algorithm for SWT on quantum computer is presented. In Section 5, a test of the quantum algorithm for SWT on a discrete version of two-site single impurity Anderson model (SIAM) is done analytically. This will be followed by a test on a general version of SIAM analytically in Section 6. After that these two models will be simulated on a quantum computer provided by IBM Qiskit and the results will be shown in Section 7. Finally we shall summarise and conclude in Section 8.

2 Schrieffer-Wolff Transformation

In this section we shall briefly introduce SWT and review some progress in the direction of its generalization. Unitary transformations are the typical methods for diagonalization in quantum mechanics as well as condensed matter physics [31]. In the unitary transformation one goes to the basis where the given Hamiltonian turns out to be diagonal. This leads to diagonalization as single step process. However, such process is impossible for every Hamiltonian. Thus in the foregoing case one attempts diagonalization of the Hamiltonian by a perturbative way. It is still possible to employ unitary transformation to do diagonalization of difficult Hamiltonians. SWT is one very important method to tame such Hamiltonians. It not only does diagonalization of the Hamiltonian by a perturbative way in that case it behaves as a unitary perturbation theory but it also does renormalization of the the parameters present in the Hamiltonian and thus can manifest itself as a type of renormalization method. SWT in the foregoing sense is employed to obtain an effective Hamiltonian for the given Hamiltonian and thus leads us to a special region of a Hamiltonian within its parameter space. It is precisely the way SWT was first applied in [6]. SWT as discussed above can be used as a unitary transformation. Thus finding an appropriate
unitary operator is vital that could either completely diagonalize the Hamiltonian or to a
desired order of perturbation.

\[ H' = U^\dagger HU \quad H' = e^SHe^{-S}. \]  

(1)

Here S represents the generator of the transformation. It is an anti-Hermitian operator.
Normally one desires of this unitary transformation to nullify the off-diagonal terms up to
the first order by satisfying the condition as given below.

\[ [S, H_0] = H_v. \]  

(2)

On elaborating the operator exponential by BCH formula one obtains series expansion
pertaining to the transformed Hamiltonian \( H' \) as follows

\[ H' = H_0 + \frac{1}{2}[S, H_v] + \frac{1}{3}[S, [S, H_v]] + ... \]  

(3)

Here \( H_0 \) and \( H_v \) are diagonal and off-diagonal pieces of the Hamiltonian \( H \) respectively.
As the off-diagonal piece is nullified up to the first order, thus the effective Hamiltonian
up to the second order turns out to be

\[ H_{\text{eff}} = H_0 + \frac{1}{2}[S, H_v]. \]  

(4)

SWT has become very significant transformation since the day it was first proposed few
decades ago. Due to this reason it has been generalized in different ways. One remarkable
generalization has been done by Wegner [32] as well as Glazek and Wilson [40] independ-
ently. The new procedure has been named by Wegner as Flow Equation Method whereas
it has been labelled as Similarity Renormalization by Glazek and Wilson. The unitary
transformation is again employed in Flow Equation Method. However, it is performed in
a continuous way as the generator relies upon the flow parameter. The connection of SWT
with Flow Equation Method has been illuminated in [41]. The generalization of SWT has
been extended to dissipative quantum systems recently [42].

Moreover, the procedure of SWT that has been discussed so far uses a generator to
accomplish the transformation. There exists a method for carrying out the transformation
where one employs Projection operators [43] or Hubbard operators [9]. Utilizing projection
operator method one gets the effective Hamiltonian. However, it fails to reproduce every
term that one obtains in SWT or generator method. Projection operator can be considered
in line with SWT due to its renormalization character where as Hubbard operator method
is specifically applicable to Hubbard model. As is evident in the above discussion for
evaluating \( H_{\text{eff}} \) one needs to find a generator that is very crucial and lies at the heart
of SWT or generator method. It is natural to have a systematic method for finding such an
SWT generator. This is precisely the subject matter of the next section.

3 Systematic Method for Schrieffer-Wolff Transformation

In this section we shall try to briefly review the progress in the development of systematic
methods for doing Schrieffer-Wolff Transformation both analytically and quantum computa-
tionally.

In [1], a new systematic method for finding generator used in doing SWT has been
reported. This analytic method is simple yet powerful. The method leads to the required
generator for SWT by just following the two steps as mentioned below
In the first step commutator \([H_o, H_v]\) is evaluated and named as \(\eta\), where \(H_o\) and \(H_v\) denote the diagonal and off-diagonal part of a given Hamiltonian \(H\) respectively.

In the second step condition is applied on \(\eta\) for removing its off-diagonal part up to first order. In order to do that coefficients are kept undetermined and are then determined by above condition. \(\eta\) is supposed to satisfy \([\eta, H_o] = -H_v\) to be the generator of the transformation. The preceding constraint identifies the coefficients and one gets the generator for SWT of the desired Hamiltonian.

This systematic method has been used to evaluate the generator of SWT for the classic model SIAM, in which SWT was employed for the first time [6]. Moreover, the calculation of generator for doing SWT to other models like Periodic Anderson Model, Anderson Holstein Model, Frohlich Hamiltonian and Jaynes-Cummings Model has been done analytically showing the utility and versatility of this novel and elegant method [1]. A question naturally arises. If we have now a systematic method that can find generator for SWT analytically, should not we have algorithms that can do SWT on quantum computer to make life even easier. As the fault-tolerant universal computer [44, 45] might not be possible in immediate future, noisy intermediate-scale quantum (NISQ) hardwares are feasible options for applications in different fields that include many-body quantum physics [46]. Beginning with the Variational Quantum Eigensolver (VQE) [47], that’s a Variational Quantum Algorithm (VQE) [48] to evaluate by employing shallow circuits the ground state of a desired Hamiltonian, various beneficial quantum algorithms for NISQ hardware have been put forward [49, 50, 51, 52]. Very recently [53] have reported some more progress in this direction. In that paper, the authors have proposed a quantum algorithm for realising SWT. They have also proposed a hybrid quantum-classical algorithm for determining the effective Hamiltonian on a hardware available in NISQ era and have applied the algorithm for Heisenberg model.

However, we don’t yet have a full fledged general quantum algorithm for SWT that can be directly implemented on quantum computer irrespective of the model under consideration. To fill this gap, we have developed one such quantum algorithm that can be directly implemented on quantum hardware. This quantum algorithm is inspired by the systematic method [1] and is discussed in the next section.

4 Quantum Algorithm for SWT

In this section we shall spell out SWT as a quantum algorithm for a general many body Hamiltonian that can be directly implemented on a quantum computer. The quantum algorithm for SWT is given in the following steps.

1. First step is to choose a desired many-body Hamiltonian \(H\) for which SWT has to be simulated on a quantum computer.

2. Then the fermionic operators in the chosen Hamiltonian have to be written in a language that quantum computer understands. This language is qubit language. That means in other words writing fermionic operators as unitary operators that can be used as quantum gates on a quantum computer. For that one has to map the fermionic operators to qubit operators like for example Pauli strings. Many such mappings are available like Jordan-Wigner(JW) Mapping, Brayvi-Kitaev Mapping and Parity mapping to name a few.

3. Once we have converted the chosen Hamiltonian in qubit language by a particular mapping, we can write qubit Hamiltonian mathematically as follows

\[
H = H_q
\]
where $H_q$ is the chosen Hamiltonian in the qubit language.

4. Now the qubit Hamiltonian obtained in Eq. (5) can be dissected into two parts, viz., diagonal part and an off-diagonal part as follows

$$H_q = H_q^o + H_q^v$$

(6)

where, $H_q^o$ and $H_q^v$ denote the diagonal and off-diagonal part of qubit Hamiltonian $H_q$ respectively. All terms of diagonal part and an off-diagonal part commute within themselves but not across.

5. After that one can proceed for an evaluation of the ansatz as proposed in [1]. This ansatz makes life easier by finding the generator for SWT systematically in the qubit language and is determined by the following commutator

$$\eta_q = [H_q^o, H_q^v].$$

(7)

At this stage $\eta_q$ gives the form of $S_q$, that is, qubit generator for quantum SWT with unknown coefficients.

6. To get the final form of $S_q$ obtained in previous step with known coefficients, it needs to be processed further so that coefficients are determined. For that an evaluation of the following commutator is required

$$[S_q, H_q^o] = -H_q^v.$$  

(8)

The above constraint helps one to obtain the required qubit generator with known coefficients needed for quantum simulation of SWT.

7. Finally we employ the quantum generator $S_q$ evaluated at the end of step 6 in the second term of the effective qubit Hamiltonian as follows

$$H_q^{eff} = H_q^o + \frac{1}{2} [S_q, H_q^v].$$

(9)

Where $H_q^{eff}$ is the required effective qubit Hamiltonian up to second order.

In the following sections our concern will be to implement this algorithm. First we shall describe it analytically followed by implementation on quantum simulator. To demonstrate all this we need to take a prototypical model. One such model is the SIAM. So we discuss it analytically in the next section by taking first a simpler version of it.

## 5 Analytical Calculations to Test Quantum SWT Algorithm

It would be appropriate at this point to demonstrate analytically the quantum SWT algorithm proposed in previous section on a simple model. The first step would be then to choose one such model. In this section we shall do analytical calculations for quantum SWT generator and calculate qubit effective Hamiltonian up to second order $H_q^{eff}$ for a simple version of SIAM that consists of one electron in conduction band and one in impurity level. The Hamiltonian for this 2-site model looks like the following

$$H = U n_{1\downarrow} n_{1\uparrow} - \mu \sum \sigma n_{1\sigma} + \sum \sigma \epsilon_2 c_2^\dagger \sigma c_2^\sigma + \sum \sigma V (c_1^\dagger \sigma c_2^\sigma + c_2^\dagger \sigma c_{1\sigma}).$$

(10)

Now according to Step 2 of the quantum SWT algorithm, we need to map this Hamiltonian to qubit language by using any of the qubit mappings available. Here we use JW mapping and the Hamiltonian in qubit language turns out to be the following.
\[ H_q = \frac{U}{4} \sigma_i^x \sigma_i^z + \left( \frac{\mu}{2} - \frac{U}{4} \right) (\sigma_i^+ \sigma_i^-) - \frac{\epsilon_2}{2} (\sigma_i^z + \sigma_i^\dagger) + \frac{V}{2} (\sigma_i^+ \sigma_i^z + \sigma_i^y \sigma_i^y + \sigma_i^z \sigma_i^x + \sigma_i^\dagger \sigma_i^y). \] (11)

So now onwards as per the quantum algorithm for SWT as spelled out in the last section we proceed as follows. First we split the above qubit Hamiltonian into diagonal and off-diagonal parts as given below

\[ H_q = H^o_q + H^v_q \] (12)

where

\[ H^o_q = \frac{U}{4} \sigma_i^x \sigma_i^z + \left( \frac{\mu}{2} - \frac{U}{4} \right) (\sigma_i^+ \sigma_i^-) - \frac{\epsilon_2}{2} (\sigma_i^z + \sigma_i^\dagger) \] (13)

and

\[ H^v_q = \frac{V}{2} (\sigma_i^z \sigma_i^x + \sigma_i^y \sigma_i^y + \sigma_i^z \sigma_i^x + \sigma_i^\dagger \sigma_i^y). \] (14)

Next step is to calculate \( \eta_q \). For that we need to evaluate the following commutator

\[ \eta_q = [H^o_q, H^v_q]. \] (15)

Using Eq.(13) and Eq.(14), the commutator turns out to be as follows

\[ \eta_q = \frac{iUV}{4} (\sigma_i^z (\sigma_i^y \sigma_i^x - \sigma_i^x \sigma_i^y) + \sigma_i^z (\sigma_i^y \sigma_i^x - \sigma_i^x \sigma_i^y)) + (iV (\frac{\mu}{2} - \frac{U}{4}) + \frac{i\epsilon_2}{2} V) (\sigma_i^y \sigma_i^x - \sigma_i^x \sigma_i^y + \sigma_i^y \sigma_i^x - \sigma_i^x \sigma_i^y). \] (16)

According to the quantum SWT algorithm, the above equation suggests the form of the qubit generator \( S_q \) for SWT as follows

\[ S_q = A(\sigma_i^y \sigma_i^x - \sigma_i^x \sigma_i^y)(1 - \sigma_i^z) + B(\sigma_i^y \sigma_i^x - \sigma_i^x \sigma_i^y)(1 - \sigma_i^z). \] (17)

To determine the coefficients A and B, the constraint as given in Step 6 of the quantum algorithm has to be applied as follows

\[ [S_q, H^o_q] = -H^v_q. \] (18)

Using Eq.(13), Eq.(14) and Eq.(17) in above constrain and then after evaluation, we get

\[ A = \frac{-iV}{4U(1 - \sigma_i^z)}, \] (19)

\[ B = \frac{-iV}{4U(1 - \sigma_i^z)}. \] (20)

Once we know \( S_q \) completely, the last step of calculating \( H^{eff}_q \) up to second order is straightforward. We only need to plug in the following commutator result in the second term of \( H^{eff}_q \) of Eqn.(9)

\[ [S_q, H^v_q] = \frac{V^2}{4U} (2(\sigma_i^z + \sigma_i^\dagger) - 2(\sigma_i^2 + \sigma_i^\dagger)). \] (21)

This completes analytically the demonstration of quantum algorithm for SWT on the simple version of 2-site SIAM. It can be extended to multiple electrons in the conduction band and forms the subject matter of the next section.
6 Quantum Algorithm for Anderson Impurity Model

In this section we shall do analytical calculations for quantum SWT generator and calculate qubit effective Hamiltonian up to second order $H_f^{eff}$ for a multiple site SIAM in 1 dimension. The Hamiltonian for this $N$-site model looks like the following

$$H = \sum_{i=1}^{N} V_i (c_{i\sigma} c_{i\sigma}^\dagger + c_{i\sigma}^\dagger c_{i\sigma}) + U n_{0\uparrow} n_{0\downarrow} + \sum_{i=0,\sigma}^{N} (\epsilon_i - \mu) n_{i\sigma}. \quad (22)$$

The JW mapping allows us to transform the fermionic Hamiltonian into the following qubit language

$$H_q = \sum_{i=1}^{N} \frac{V_i}{2} (X_0 Z_1...Z_{i-1}X_i + Y_0 Z_1...Z_{i-1}Y_i + X_{N+1} Z_{N+2}...Z_{N+i}X_{N+1+i} + Y_{N+1} Z_{N+2}...Z_{N+i}Y_{N+1+i}) + U/4 (Z_0 Z_{N+1} - Z_0 - Z_{N+1}) + \sum_{i=0}^{N} (\epsilon_i - \mu/2) (Z_i + Z_{N+1+i}). \quad (23)$$

Now we shall split the above qubit Hamiltonian into diagonal and off-diagonal parts as given below

$$H_q^0 = \frac{U}{4} (Z_0 Z_{N+1} - Z_0 - Z_{N+1}) + \sum_{i=0}^{N} (\epsilon_i - \mu/2) (Z_i + Z_{N+1+i}), \quad (24)$$

$$H_q^v = \sum_{i=1}^{N} \frac{V_i}{2} (X_0 Z_1...Z_{i-1}X_i + Y_0 Z_1...Z_{i-1}Y_i + X_{N+1} Z_{N+2}...Z_{N+i}X_{N+1+i} + Y_{N+1} Z_{N+2}...Z_{N+i}Y_{N+1+i}). \quad (25)$$

To calculate $\eta_q$, we need to evaluate the following commutator

$$\eta_q = [H_q^0, H_q^v]. \quad (26)$$

Using Eq.(24) and Eq.(25), the above commutator takes the following form

$$\eta_q = 2i (\frac{U}{4} + (\epsilon_0 - \mu)/2 + (\epsilon_0 - \mu)/2) \sum_{i=1}^{N} \frac{V_i}{2} (Z_1...Z_{i-1}(Y_i X_0(1-Z_{N+1}) - X_i Y_0(1-Z_{N+1})) + Z_{N+2}...Z_{N+i}(Y_{N+1+i} X_{N+1}(1-Z_0) - X_{N+1+i} Y_{N+1}(1-Z_0))). \quad (27)$$

The above expression implies the form of the qubit generator $S_q$ for SWT as follows

$$S_q = \sum_{i=1}^{N} (AZ_1...Z_{i-1}(Y_i X_0(1-Z_{N+1}) - X_i Y_0(1-Z_{N+1})) + B Z_{N+2}...Z_{N+i}(Y_{N+1+i} X_{N+1}(1-Z_0) - X_{N+1+i} Y_{N+1}(1-Z_0))). \quad (28)$$

To find the coefficients A and B, the following SWT condition has to be followed

$$[S_q, H_q^0] = -H_q^v. \quad (29)$$
Employing Eq.(24), Eq.(25) and Eq.(28) in above condition gives

\[
A = \frac{-iV}{4U(1 - Z_{N+1})},
\]

\[
B = \frac{-iV}{4U(1 - Z_0)},
\]

and thus our required generator takes the following form

\[
S_q = \sum_{i=1}^{N} \frac{-iV}{4U} (Z_i...Z_{i-1}(Y_iX_0 - X_iY_0) + Z_{N+2}...Z_{N+i}(Y_{N+1+i}X_{N+1} - X_{N+1+i}Y_{N+1})).
\]

After finding \(S_q\) the final step of evaluating \(H_{\text{eff}}^q\) up to second order is given by using following commutator result in the second term of \(H_{\text{eff}}^q\) of Eqn.(9)

\[
\left[ S_q, H_q^v \right] = \sum_{i=1}^{N} \frac{V^2}{4U} (Z_i...Z_{i-1}(-2Z_i - 2Z_0)).
\]

This completes the analytical demonstration of quantum algorithm for SWT of multiple electrons in the conduction band of SIAM. Verifying this quantum algorithm for SWT experimentally for various cases is the next important stage and is discussed in the following section.

7 Experiments on IBM Quantum Devices

We implemented our quantum algorithm for SWT in Qiskit and did the experiments on IBM Quantum computers. In this section, we give the details of the our experiments and the results. The Qiskit code snippets for various steps of the quantum algorithm have also been included. These figures are for the case of 2-site(4 qubit) SIAM. The results for 8 qubit SIAM are given in the Appendix A.

Figure 1: 4 qubit Hamiltonian after Jordan-Wigner Mapping of 2-site SIAM Hamiltonian.
8 Conclusion and Discussion

Schrieffer-Wolff transformation is extensively used in diverse areas of quantum many-body physics including quantum condensed matter physics, quantum optics, quantum electrodynamics and has found applications in quantum complexity theory. This transformation is routinely used by researchers to calculate the low energy effective Hamiltonians corresponding to interesting fixed points which arise due to the effect of strong correlations in these systems. Therefore, it becomes natural to have quantum algorithm for carrying out Schrieffer-Wolff transformation on quantum computer. In this work, we have demonstrated such an algorithm and have reproduced the historical mapping of Anderson impurity model
to Kondo model which was shown in the very first application of SWT. Our quantum algo-
rithm is not restricted to Anderson impurity model, rather it can applied to a broad class
of quantum many-body Hamiltonians which share similar structure to Anderson Impurity
model. We hope our work will open up new directions for carrying out SWT for various
quantum many-body models using quantum computers.

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A First section of the appendix

Figure 5: Jordan-Wigner Mapping code for 8 qubit Hamiltonian of 4-site SIAM.

Qubit Hamiltonian of AIM is:
0.125 * IIIIIIIY
+ 0.125 * IIIIIIXX
+ 0.125 * IIIIYZZY
+ 0.125 * IIIIXZX
+ 0.125 * IYYIII
+ 0.125 * IIIXXIX
+ 0.125 * IYZZYIII
+ 0.125 * IXZIXIII
+ 0.125 * YZZYIII
+ 0.125 * XXZXIII
+ 1.359999999999994 * IIIIIII
- 1.045 * IIIZIIII
- 1.045 * IIIIIIIZ
+ 1.0 * IIIZIIIZ
- 0.045 * IIIIIIZI
- 0.045 * IIIIIIZII
- 0.045 * IIIIZIII
- 0.045 * IIZIII
- 0.045 * IIIZIII
- 0.045 * ZZIIIII
- 0.045 * ZIIIII

Figure 6: 8 qubit Hamiltonian after Jordan-Wigner Mapping of 4-site SIAM Hamiltonian.
Figure 7: Code for $\eta_q = [H_q^0, H_q^v]$ for 8 qubit Hamiltonian of 4-site SIAM Hamiltonian.

$$\eta_q = [H_q^0, H_q^v]$$

Figure 8: $\eta_q = [H_q^0, H_q^v]$ for 8 qubit Hamiltonian of 4-site SIAM Hamiltonian.

$$\eta_q = [H_q^0, H_q^v]$$
Figure 9: Commutator $[S_q, H^0_q]$ for 8 qubit Hamiltonian of 4-site SIAM Hamiltonian.

Figure 10: 8 qubit Effective Hamiltonian $H^e_{q}$ for 4-site SIAM Hamiltonian after SWT.
Figure 11: Remaining part of 8 qubit Effective Hamiltonian $H_{eff}^4$ for 4-site SIAM Hamiltonian after SWT.
Figure 12: Remaining part of 8 qubit Effective Hamiltonian $H_q^{eff}$ for 4-site SIAM Hamiltonian after SWT.
Figure 13: Remaining part of 8 qubit Effective Hamiltonian $H^{eff}_4$ for 4-site SIAM Hamiltonian after SWT.

\[
\begin{align*}
+ & 0.001953125 \times IYXIIIYX \\
- & 0.001953124999999998 \times IXYIIYX \\
+ & 0.001953126 \times IYXIIIYX \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXYIIIXY \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999996 \times IXYIIIXY \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
- & 0.001953124999999998 \times IXZIIIXX \\
+ & 0.001953126 \times IIXXIIXY \\
- & 0.001953124999999996 \times IXZIIIXX \\
+ & 0.001953126 \times IYXIIIXY \\
\end{align*}
\]

Figure 14: Remaining part of 8 qubit Effective Hamiltonian $H^{eff}_4$ for 4-site SIAM Hamiltonian after SWT.

\[
\begin{align*}
- & 0.001953125 \times IYZXZXY \\
+ & 0.001953124999999996 \times IXYZXZY \\
- & 0.001953126 \times IYZXZXY \\
+ & 0.001953124999999996 \times IXYZXZY \\
\end{align*}
\]