EQUIVALENT TWO-BODY FORCES FOR MANY-BODY PROBLEMS WITH THREE-BODY FORCES

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A thesis submitted in partial fulfillment
of the requirements for the degree of
Master of Science

Department of Physics

Central Michigan University
Mount Pleasant, Michigan
August 2011

Accepted by the Faculty of the College of Graduate Studies,

Central Michigan University, in partial fulfillment of

the requirements for the master's degree

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I dedicate this work to my parents,
for all their support
throughout this work.

ACKNOWLEDGMENTS

I would like to thank my thesis advisor Dr. Mihai Horoi for his invaluable support during the development of this thesis. Without his support it would be impossible for me to finish this thesis. I would also like to thank other members of thesis committee: Dr. Stanley Hirschi, and Dr. Marco Fornari. These faculty members provided valuable direction when this project began, reviewed the draft of the document, and made many contributions to the final product. I thank Dr. Mihai Horoi, and Dr. Koblar Alan Jackson. I have taken Quantum mechanics classes from them and without their help I would not be able to do my research in this area. Finally, I want to thank my parents for their moral support and their best wishes for me in every step of my life.

ABSTRACT

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by Animesh Sarker

Physical world consists of many particles, and then there are interactions among those particles. An exact solution of Schrodinger equation for many particle systems is unknown. But the "second quantization" is a technique that greatly simplifies the calculations for many-body interaction, for both relativistic and non-relativistic cases. In second quantization, the many body Hamiltonian for bosons or fermions constitutes 2-body, 3-body, 4-body interactions and more. In this thesis, we will find equivalent 2-body interactions for k-body interactions for a system of n bosons or n fermions. By adding all these 2-body interactions we will get a 2-body effective Hamiltonian, which will approximate the ground state energy of the exact Hamiltonian. Quantum computer is a device that uses the principles of quantum mechanics. And a qubit is the smallest unit of information in quantum computers that is the quantum analog of classical bit. In quantum computation, Sergey Bravyi and collaborators has developed a technique to find a 2-body effective Hamiltonian for a k-body Hamiltonian acting on n-qubits. We applied this idea for a system of n fermions or n bosons and found an equivalent 2-body effective Hamiltonian for the Hamiltonian of bosons or fermions.

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KEYS TO SYMBOLS

$\mathbb{R}$	the set of real numbers
$\mathbb{C}$	the set of complex numbers
δ_{ij}	Kronecker symbol
$\|\|x\|\|$	the norm of a vector x
x^*	complex conjugate of x
$\|\|T\|\|$	the norm of an operator T
$C[a,b]$	the space of continuous real valued functions on $[a,b]$
$O(f(x))$	$f(x)$ is bounded above by $K \cdot O(f(x))$ as $x \to \infty$ for some constant K
$\langle x\|T\|y\rangle$	the inner product of vectors x and Ty
$\sigma_x, \sigma_y, \sigma_z$	Pauli X, Y, Z operators/matrices
$A \otimes B$	Tensor product of A and B

CHAPTER I

INTRODUCTION

Quantum mechanics is a theory of physics which can successfully explain the behavior of electrons, protons, atoms, molecules, nuclei and other tiny particles. Classical mechanics uses Newton's laws of motion to describe the behavior of a particle. Though the Newton's laws of motion are successful in describing the properties in a macroscopic level, they are not adequate to explain properties in a microscopic level. Quantum mechanics takes a completely different approach to describe the behavior of particle which are no larger than typical size of a molecule. Quantum mechanics uses wave functions and these wave functions are the solutions of Schrödinger equation. The Schrödinger equation in quantum mechanics plays the role of Newton's laws in classical mechanics. Schrödinger equation is a second order partial differential equation. For most of the quantum mechanical problems, it is impossible to solve this equation analytically. Therefore we need numerical techniques as well as some approximation techniques to solve the Schrödinger equation for realistic systems.

Physical world consists of many particles as well as the interactions among those particles. Exact solution of Schrödinger equation for many particle system is unknown. Second quantization is a technique which is used to deal with many particle system. Second quantization greatly simplifies the calculations for many-body interaction for both relativistic and non-relativistic cases. The second quantized form of Hamiltonian contains two operators called annihilation operator and creation operator. The many body Hamiltonian for bosons or fermions in second quantization takes the form

$$H = H_1 + H_2 + H_3 + \cdots \tag{I.1}$$

where H_k is an operator that contains the product of k annihilation operators and creation operators. More explicitly, H_k can be written as $\sum\langle i_1 \cdots i_k \mid V \mid j_1 \cdots j_k\rangle b^\dagger_{i_1} \cdots b^\dagger_{i_k} b_{j_1} \cdots b_{j_k}$ for bosons and $\sum\langle i_1 \cdots i_k \mid V \mid j_1 \cdots j_k\rangle a^\dagger_{i_1} \cdots a^\dagger_{i_k} a_{j_1} \cdots a_{j_k}$ for fermions and therefore, H_k contains all k-body interactions. In this expression $b^\dagger_{i_k}$ and $a^\dagger_{i_k}$ are the creation operators for bosons and fermions respectively and b_{i_k} and a_{i_k} are the annihilation operators for bosons and fermions respectively. Annihilation operators and creation operators act on subspaces of Fock space. Our goal is to replace k-body interactions by 2-body interactions and write a 2-body effective Hamiltonian which approximates some of the properties of the exact Hamiltonian. In this thesis, we will construct a 2-body effective Hamiltonian such that the effective Hamiltonian approximates the ground state energy of the exact Hamiltonian.

The idea of approximating the exact Hamiltonian by a 2-body effective Hamiltonian is not new. Dirac pointed out that in hydrogen molecule the important features about spin interactions could be obtained by a potential of form $-2J_{ab}\bar{s_a} \cdot \bar{s_b}$, where J_{ab} is the exchange constant and $\bar{s_a}$ and $\bar{s_b}$ are the spin momenta. This expression is called the Heisenberg exchange Hamiltonian or Heisenberg-Dirac Hamiltonian. Heisenberg exchange Hamiltonian gives the exchange interaction between two electrons in orbitals ϕ_a and ϕ_b. Exchange interactions are very short-ranged. This interaction is usually confined to nearest neighbors. In crystal, the exchange interaction takes the form

$$H_{\text{Heis}} = -\sum_{i,j} J_{ij} \bar{S}_i \cdot \bar{S}_j \tag{I.2}$$

Heisenberg Hamiltonian assumes the localized exchange coupling of electrons. Therefore it is a successful model for explaining magnetic properties of electrically insulating narrow-band ionic and covalent non-molecular solid. But the electrons, which are responsible for ferromagnetism in some non-molecular solids like iron, nickel etc., are not localized. Heisenberg model is not adequate to explain the ferromagnetism in these metals. The Ising model of ferromagnetism is similar to Equation (I.2) except it uses the scalar product of z-component of spin instead of dot product.

$$E = -\sum_{i \neq j} J_{ij} S_i^z S_j^z \tag{I.3}$$

The motivation of Ising came from the phenomenon of ferromagnetism. Once Iron is magnetized, it remains magnetized for long time. Ferromagnetism can be explained by the spin property of electron. Ferromagnetic materials show ferromagnetism because large number of electrons spin in the same direction. An electron on one side of a material doesn't know the direction of the spin of the electron on the other side. It can interact with only with its neighbor electrons. This is the main idea behind the Ising model.

Quantum computer is a device which uses the principles of quantum mechanics. In quantum computation, a 2-body effective Hamiltonian is derived for a k-body effective Hamiltonian acting on n qubits [2]. A Qubit is the quantum analog of bit which has two stationary states $|0\rangle$ and $|1\rangle$. A k-body Hamiltonian is a Hamiltonian $H = H_1 + H_2 + \cdots$ where H_i is a Hermitian operator acting on no more than k particles. To find a 2-body effective Hamiltonain, the authors in [2] used two gadgets called subdivision gadget and 3-to-2 gadget. Gadget is a technical term and it means an extra qubits which is used to perform a specific job. Subdivision gadget is used to decompose a k-body target (or exact) Hamiltonian of form $H_{\text{target}} = JAB$ where A and B are operators acting on $\lceil k/2 \rceil$ or $\lfloor k/2 \rfloor$ disjoint subsets of qubits and J is a constant. After applying subdivision gadget we get an effective Hamiltonian $H_{\text{eff}} = H_{\text{eff1}} + H_{\text{eff2}}$ where H_{eff1} contains A but not B and H_{eff2} contains B but not A. Since one extra qubit is added to the system, H_{eff} is a $\lceil k/2 \rceil + 1$-body Hamiltonian. By using subdivision gadget several times we get a 3-body effective Hamiltonian. Then 3-to-2 gadget is used to transform a 3-body Hamiltonian $H_{\text{target}} = JABC$ to a 2-body Hamiltonian where A, B, C act on different qubits. The effective Hamilatonians for subdivision gadget and 3-to-2 gadget were derived for an operator of form

$H_{\text{target}} = JAB$ and $H_{\text{target}} = JABC$ where A, B, and C act on different subsets of qubits and so they commute. Commutativity is the main property that was used in the proof of these two gadgets.

We were inspired by the technique used to find a 2-body effective Hamiltonian for a k-body target Hamiltonian acting on n qubits. We applied this technique for the Hamiltonian of bosons and fermions to find a 2-body effective Hamiltonian. Each term H_i in equation I.1 can be written as $JABC\cdots$ such that $A,B,C,\cdots$ are one particle operators. Since the operators $A,B,C,\cdots$ may not commute we need to modify the subdivision gadget so that we can apply it for non-commuting operators. Then we apply these gadgets on the Hamiltonian for bosons and fermions to find an effective Hamiltonian.

We divide this thesis into four different chapters. We give a brief introduction in chapter I. In chapter II, we will discuss the basic concepts which are required to understand the main problem and the solution. We will discuss about the second quantization of fermions and bosons in this chapter. We will also give a brief introduction of quantum computation. Quantum computers work with the system of qubits. Since tensor product space is the mathematical model for a system of qubits we will discuss about the tensor product and tensor product space in this chapter. We will explain the basic ideas behind quantum algorithm and finally we will discuss some of the quantum gates which are used in quantum computers.

We will present our main results in chapter III. Our main results include the following.

- Extension of the subdivision gadget presented in [2] for non-commutative operators.
- constructing a 2-body effective Hamiltonian for the Hamiltonian of bosons and fermions.

We will give a conclusion of this thesis in chapter IV.

CHAPTER II

SECOND QUANTIZATION AND QUANTUM COMPUTATION

In this chapter we will give brief introduction to two important topics: second quantization and quantum computation. To find a two body Hamiltonian for fermions or bosons, we used the second quantized form of Hamiltonian. But the main idea to solve this problem comes from quantum computation. After introducing these two topics in this chapter, we will discuss about finding two body Hamiltonian in next chapter.

II.1 Second Quantization

In second quantization the Hamiltonian of bosons and fermions take the following forms.

$$\begin{aligned}
H_{\text{boson}} &= \sum_{i,j} \langle i \mid V \mid j \rangle b_i^\dagger b_j + \sum_{i,j,k,l} \langle ij \mid V \mid kl \rangle b_i^\dagger b_j^\dagger b_k b_l \\
&+ \sum_{i,j,k,l,m,n} \langle ijk \mid V \mid lmn \rangle b_i^\dagger b_j^\dagger b_k^\dagger b_l b_m b_n + \cdots \\
H_{\text{fermion}} &= \sum_{i,j} \langle i \mid V \mid j \rangle a_i^\dagger a_j + \sum_{i,j,k,l} \langle ij \mid V \mid kl \rangle a_i^\dagger a_j^\dagger a_k a_l \\
&+ \sum_{i,j,k,l,m,n} \langle ijk \mid V \mid lmn \rangle a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n + \cdots
\end{aligned}$$

where $b_i^\dagger$, b_j are the creation operator and the annihilation operator of bosons and $a_i^\dagger$, a_j are the creation operator and the annihilation operator of fermions. These operators are used to create and annihilate particles in a system of bosons or fermions. In the Hamiltonian of bosons or fermions, the term which involves $b_i^\dagger b_j^\dagger b_k b_l$ is a two body interaction, the term which involves $b_i^\dagger b_j^\dagger b_k^\dagger b_l b_m b_n$ is a three body interaction and so on. Our goal is to consider each term separately and approximate them by two body interactions to get a 2-body effective Hamiltonian. Here by 'approximate' we mean that the ground state energy of the effective Hamiltonian is close to the ground state energy of the exact Hamiltonian. Using commutator or anti-commutator relation of annihilation and creation operators, we will rewrite each term as a product of operators $ABCD\cdots$ where $A,B,C,\cdots$ are one body operators of form $b_i^\dagger b_j$ or $a_i^\dagger a_j$. Then we will apply the subdivision gadget and 3-to-2 gadget to decompose these operators. This technique will be described in the next chapter in details.

II.1.1 Creation and Annihilation Operators

In many particle quantum mechanics, specially in second quantization, creation and annihilation operators play a very important role. These two operators act on a space called Fock space. The basis for Fock space consists of symmetric or antisymmetric functions. Particles that require symmetric wave function are called bosons and the particles that require antisymmetric wave function are called fermions. Symmetric and antisymmetric wave functions are represented by a convenient notation called 'occupation number representation'. If n_1 particles are in state 1, n_2 particles are in state 2, n_3 particles are in state 3 and so on, then normalized and completely symmetrized or antisymmetrized eigenfunction is written as $|n_1,n_2,n_3,\cdots)$. For fermions,

$$
\begin{aligned}
|1,1) &= \frac{1}{\sqrt{2}}(\psi_1(1)\psi_2(2)-\psi_1(2)\psi_2(1)) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_1(1) & \psi_2(1) \\ \psi_1(2) & \psi_2(2) \end{vmatrix} \\
|1,0,1) &= \frac{1}{\sqrt{2}}(\psi_1(1)\psi_3(2)-\psi_1(2)\psi_3(1)) = \frac{1}{\sqrt{2}}\begin{vmatrix} \psi_1(1) & \psi_3(1) \\ \psi_1(2) & \psi_3(2) \end{vmatrix} \\
|1,1,1) &= \frac{1}{\sqrt{6}}\begin{vmatrix} \psi_1(1) & \psi_2(1) & \psi_3(1) \\ \psi_1(2) & \psi_2(2) & \psi_3(2) \\ \psi_1(3) & \psi_2(3) & \psi_3(3) \end{vmatrix} \\
|1,2) &= 0
\end{aligned}
$$

We can always write the antisymmetric wavefunctions using a determinant. For a system of N identical particles we will start with $\Psi(1,2,3,\cdots,N) = \psi_1(1)\psi_2(2)\psi_3(3)\cdots\psi_N(N)$ and then we can antisymmetrize it using the following determinant.

$$\Psi_A(1,2,3,\cdots N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(1) & \psi_2(1) & \psi_3(1) & \cdots & \psi_N(1) \\ \psi_1(2) & \psi_2(2) & \psi_3(2) & \cdots & \psi_N(2) \\ & & \vdots & & \\ \psi_1(N) & \psi_2(N) & \psi_3(N) & \cdots & \psi_N(N) \end{vmatrix}$$

This determinant is called the Slater determinant. To get the complete symmetric wave function for bosons, we find all the permutations and then we add all those terms. For example,

$$\begin{aligned}
|1,1\rangle &= \frac{1}{\sqrt{2}}(\psi_1(1)\psi_2(2)+\psi_1(2)\psi_2(1)) \\
|1,0,1\rangle &= \frac{1}{\sqrt{2}}(\psi_1(1)\psi_3(2)+\psi_1(2)\psi_3(1)) \\
|1,1,1\rangle &= \frac{1}{\sqrt{6}}(\psi_1(1)\psi_2(2)\psi_3(3)+\psi_1(1)\psi_2(3)\psi_3(2)+\psi_1(2)\psi_2(3)\psi_3(1) \\
&+ \psi_1(2)\psi_2(1)\psi_3(3)+\psi_1(3)\psi_2(1)\psi_3(2)+\psi_1(3)\psi_2(2)\psi_3(1)) \\
|1,2\rangle &= \frac{1}{\sqrt{3}}(\psi_1(1)\psi_2(2)\psi_2(3))+\psi_1(2)\psi_2(3)\psi_2(1)+\psi_1(3)\psi_2(1)\psi_2(2) \\
&= \frac{\sqrt{2!}}{\sqrt{3!}}(\psi_1(1)\psi_2(2)\psi_2(3))+\psi_1(2)\psi_2(3)\psi_2(1)+\psi_1(3)\psi_2(1)\psi_2(2) \\
&= \frac{1}{\sqrt{2!}}\frac{2!}{\sqrt{3!}}(\psi_1(1)\psi_2(2)\psi_2(3)+\psi_1(2)\psi_2(3)\psi_2(1)+\psi_1(3)\psi_2(1)\psi_2(2) \\
&= \frac{1}{\sqrt{2!}}\frac{1}{\sqrt{3!}}(\psi_1(1)\psi_2(2)\psi_2(3)+\psi_1(1)\psi_2(3)\psi_2(2)+\psi_1(2)\psi_2(3)\psi_2(1) \\
&+ \psi_1(2)\psi_2(1)\psi_2(3)+\psi_1(3)\psi_2(1)\psi_2(2)+\psi_1(3)\psi_2(2)\psi_2(1))
\end{aligned}$$

The states $|n_1 n_2 \cdots n_N\rangle$ are orthonormal and complete. Therefore,

$$
\begin{aligned}
\langle m_1 m_2 \cdots m_N | n_1 n_2 \cdots n_N \rangle &= \delta_{m_1 n_1} \delta_{m_2 n_2} \cdots \delta_{m_N n_N} \\
\sum_{n_1, n_2, \cdots n_N} |n_1 n_2 \cdots n_N\rangle \langle n_1 n_2 \cdots n_N| &= 1
\end{aligned}
$$

Because of the orthonormality of the basis states, we have $\langle 1,2,1,1,5|1,3,1,1,5\rangle = 0$ but $\langle 1,3,1,1,5|1,3,1,1,5\rangle = 1$. Now we will define the creation operator $b_i^\dagger$ and annihilation operator b_i for bosons that act on the space whose basis states are $|n_1 n_2 \cdots n_N\rangle$. The creation and annihilation operators of bosons are defined as

$$
\begin{aligned}
b_i^\dagger |n_1, n_2, \cdots, n_i, \cdots n_N\rangle &= \sqrt{n_i + 1}\,|n_1, n_2, \cdots, (n_i + 1), \cdots n_N\rangle \\
b_i |n_1, n_2, \cdots, n_i, \cdots n_N\rangle &= \sqrt{n_i}\,|n_1, n_2, \cdots, (n_i - 1), \cdots n_N\rangle
\end{aligned}
$$

The definition of annihilation and creation operators for fermions are similar to the definition of annihilation and creation operators for bosons. The main difference is that if two fermions are in the same state then the wavefuncion vanishes. So

$$
\begin{aligned}
(a_i^\dagger)^2 |n_1, n_2, \cdots, n_i, \cdots, n_N\rangle &= 0 \qquad \text{and} \\
(a_i)^2 |n_1, n_2, \cdots, n_i, \cdots, n_N\rangle &= 0
\end{aligned}
$$

Therefore, the only possible values of n_i are 0 and 1. We can define the annihilation and creation operators for fermions as follows.

$$
\begin{aligned}
a_i^\dagger |n_1, n_2, \cdots, n_i, \cdots n_N\rangle &= \begin{cases} (-1)^{S_i} \sqrt{n_i + 1}\,|n_1, n_2, \cdots, (n_i + 1), \cdots n_N\rangle, & \text{if } n_i = 0 \\ 0, & \text{otherwise} \end{cases} \\
a_i |n_1, n_2, \cdots, n_i, \cdots n_N\rangle &= \begin{cases} (-1)^{S_i} \sqrt{n_i}\,|n_1, n_2, \cdots, (n_i - 1), \cdots n_N\rangle, & \text{if } n_i = 1 \\ 0, & \text{otherwise} \end{cases}
\end{aligned}
$$

where $S_i = n_1 + n_2 + \cdots + n_{i-1}$

Properties of annihilation and creation operator

We can use the definition to prove the following properties for creation and annihilation operators for bosons.

(a) $b_i^\dagger b_i = n_i$

(b) $[b_i, b_j^\dagger] = \delta_{ij}$

(c) $[b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0$

where the commutator is defined by $[A,B] = AB - BA$. The operator $b_i^\dagger b_i$ is called the number operator, since its eigenvalue is the number of particles in i^{th} state. The second property shows that the annihilation operator and the creation operator for different states commute but for the same state, they don't commute. The following are the properties for annihilation and creation operators for fermions.

(a) $a_i^\dagger a_i = n_i$

(b) $\{a_i, a_j^\dagger\} = \delta_{ij}$

(c) $\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0$

where the anticommutator is defined by $\{A,B\} = AB + BA$. If A and B anticommute, then $AB + BA = 0$, i.e. $AB = -BA$. The operator $a_i^\dagger a_i$ is called the number operator, because its eigenvalue is the number of particles in i^{th} state. The second property implies that the annihilation operator and the creation operator for different states anticommute but for the same state, they don't anticommute. Now we will see an example of two boson system and in this example we will also show how to find the operator norm of $b_i b_i^\dagger$ and $b_i^\dagger b_i$.

An example: two boson system

Let us consider a system of two bosons with two possible states for each boson. Then we have three possible stationary states for this system.

$$\begin{aligned}
|I\rangle &= |2,0\rangle = \frac{1}{\sqrt{2}}(b_1^\dagger)^2 \mid 0,0\rangle \\
|II\rangle &= |1,1\rangle = b_1^\dagger b_2^\dagger \mid 0,0\rangle \\
|III\rangle &= |0,2\rangle = \frac{1}{\sqrt{2}}(b_2^\dagger)^2 \mid 0,0\rangle
\end{aligned}$$

We will evaluate $\langle I \mid H \mid I\rangle$, $\langle I \mid H \mid II\rangle$, $\langle II \mid H \mid I\rangle$ and $\langle II \mid H \mid II\rangle$ for H in equation **??**.

$$\begin{aligned}
\langle 0,0 \mid (b_1)^2 b_i^\dagger b_i (b_1^\dagger)^2 \mid 0,0\rangle &= \langle 0,0 \mid b_1(\delta_{1i} + b_i^\dagger b_1)(\delta_{1i} + b_1^\dagger b_i) b_1^\dagger \mid 0,0\rangle \\
&= \langle 0,0 \mid (b_1 b_1^\dagger + b_1 b_i^\dagger b_1 b_1^\dagger + b_1 b_1^\dagger b_i b_1^\dagger + b_1 b_i^\dagger b_1 b_1^\dagger b_i b_1^\dagger) \mid 0,0\rangle \delta_{1i} \\
&= \langle 0,0 \mid (1 + b_1^\dagger b_1 + b_1 b_i^\dagger (1 + b_1^\dagger b_1) + b_1 b_1^\dagger (\delta_{1i} + b_1^\dagger b_i) \\
&+ b_1 b_i^\dagger b_1 b_1^\dagger (\delta_{1i} + b_1^\dagger b_i)) \mid 0,0\rangle \delta_{1i} \\
&= \delta_{1i} + \langle 0,0 \mid (b_1 b_i^\dagger + b_1 b_1^\dagger + b_1 b_i^\dagger b_1 b_1^\dagger) \mid 0,0\rangle \delta_{1i} \\
&= \delta_{1i} + \langle 0,0 \mid (\delta_{1i} + b_i^\dagger b_1 + 1 + b_1^\dagger b_1 + b_1 b_i^\dagger (1 + b_1^\dagger b_1)) \mid 0,0\rangle \delta_{1i} \\
&= \delta_{1i} + \delta_{1i} + \delta_{1i} + \langle 0,0 \mid (b_1 b_i^\dagger) \mid 0,0\rangle \delta_{1i} \\
&= \delta_{1i} + \delta_{1i} + \delta_{1i} + \delta_{1i} \\
&= 4\delta_{1i}
\end{aligned}$$

By the similar calculations we can show that

$$\langle 0,0 \mid (b_1)^2 b_i^\dagger b_j^\dagger b_k b_l (b_1^\dagger)^2 \mid 0,0\rangle = 4\delta_{1i}\delta_{1j}\delta_{1k}\delta_{1l}$$

Hence,

$$\begin{aligned}
\langle I \mid H \mid I \rangle &= \sum_i T_i \langle I \mid b_i^\dagger b_i \mid I \rangle + \frac{1}{2} \sum_{i,j,k,l} \langle ij|U|kl \rangle \langle I \mid b_i^\dagger b_j^\dagger b_k b_l \mid I \rangle \\
&= \sum_i T_i \left(\frac{1}{2}\right) 4\delta_{1i} + \frac{1}{2} \sum_{i,j,k,l} \langle ij|U|kl \rangle \left(\frac{1}{2}\right) 4\delta_{1i}\delta_{1j}\delta_{1k}\delta_{1l} \\
&= 2T_1 + \langle 11|U|11 \rangle
\end{aligned}$$

Similarly,

$$\begin{aligned}
\langle I \mid H \mid II \rangle &= \frac{1}{\sqrt{2}}(\langle 11|U|12 \rangle + \langle 11|U|21 \rangle) \\
\langle II \mid H \mid I \rangle &= \frac{1}{\sqrt{2}}(\langle 11|U|12 \rangle + \langle 11|U|21 \rangle)^* \\
\langle II \mid H \mid II \rangle &= \langle 12|U|21 \rangle + \langle 12|U|12 \rangle
\end{aligned}$$

Using these matrix elements we can find the eigenvalues for the system. Since the operator norm of an operator is an important issue for our work, we will show how to find the operator norm of $b_i b_j^\dagger$ and $b_i^\dagger b_j$. A. M. Sinclair proved that if a Hermitian operator H acts on a Hilbert space then its spectral radius is equal to its operator norm[14]. Recall that if an operator is bounded then it cannot increase the size of a vector more than a constant factor. The smallest c for which $||T|x\rangle|| \leq c|||x\rangle||$, gives a measure of the operator T. This measure of T is called the norm of T and it is denoted by $||T||$. Let us apply $b_1 b_1^\dagger$ on basis states.

$\langle 2,0 \mid b_1 b_1^\dagger \mid 2,0 \rangle = 3;$ $\langle 1,1 \mid b_1 b_1^\dagger \mid 2,0 \rangle = 0;$ $\langle 0,2 \mid b_1 b_1^\dagger \mid 2,0 \rangle = 0;$

$\langle 2,0 \mid b_1 b_1^\dagger \mid 1,1 \rangle = 0;$ $\langle 1,1 \mid b_1 b_1^\dagger \mid 1,1 \rangle = 2;$ $\langle 0,2 \mid b_1 b_1^\dagger \mid 1,1 \rangle = 0;$

$\langle 2,0 \mid b_1 b_1^\dagger \mid 0,2 \rangle = 0;$ $\langle 1,1 \mid b_1 b_1^\dagger \mid 0,2 \rangle = 0;$ $\langle 0,2 \mid b_1 b_1^\dagger \mid 0,2 \rangle = 1;$

Hence the matrix representation of operator $b_1 b_1^\dagger$ is $T = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. Since the maximum eigenvalue of T is 3, the spectral radius of T is 3. Therefore the operator norm of $b_1 b_1^\dagger$ is also 3. Similar calculation shows that if $i \neq j$ then the operator norm of $b_i b_i^\dagger$, $b_i^\dagger b_i$, $b_i^\dagger b_j$, and $b_i b_j^\dagger$ are 3, 2, 2 and 0 respectively.

Remark II.1.1. *In general, we can show that if there are n particles in a system then the operator norm of $b_i b_i^\dagger$ is $n+1$ and the operator norm of $b_i^\dagger b_i$ is n.*

II.2 Quantum Computation

In recent years, physicists are showing lots of interest in the area of quantum computation. Quantum computing blossomed when Peter Shor published the factoring algorithm in 1994 [12]. Finding the prime factors of an integer is very important for the system of public key encryption. Many interesting algorithms have been developed for the conventional computers for finding the prime factors of an integer. The complexity of all these algorithms are exponential. In contrast, the complexity of Shor's algorithm for finding the prime factors of an integer is polynomial. More specifically, the time required to factor an integer N is $O((\log N)^3)$. Shor's algorithm opened a new door in complexity theory. After the factoring algorithm was published, many other interesting theories and algorithms has been developed for quantum computers, though the physical realization of quantum computer is still not clear. Qubit is the basic building block of quantum computers. A qubit has two stationary states, $|0\rangle$ and $|1\rangle$. A qubit can also be in any superposition state. When we work with a system of n qubits, then we deal with a space called tensor product space. We will briefly discussion about the tensor product and tensor product space in the following section.

II.2.1 Tensor Product and Tensor Product Space

Let X and Y are two finite dimensional vector spaces over a field K. Suppose $\{|e_1\rangle, \cdots, |e_l\rangle\}$ and $\{|f_1\rangle, |f_2\rangle, \cdots, |f_m\rangle\}$ are the bases of X and Y respectively. Define a vector space $X \otimes Y$ whose basis contains the elements of form $|e_i\rangle \otimes |f_j\rangle$, i.e. the basis of this vector space is

$$\{e_i \otimes f_j : i = 1, \cdots, l; j = 1, \cdots, m\}$$

The space $X \otimes Y$ is called a tensor product space. The tensor product of arbitrary two vectors, $|x\rangle = \sum_i x_i |e_i\rangle$ and $|y\rangle = \sum_j y_j |f_j\rangle$ is

$$|x\rangle \otimes |y\rangle = \sum_{i,j} (x_i y_j) |e_i\rangle \otimes |f_j\rangle$$

In the tensor product space $X \otimes Y$ we have the following equalities.

$$\begin{aligned}
(|x_1\rangle + |x_2\rangle) \otimes |y\rangle &= |x_1\rangle \otimes |y\rangle + |x_2\rangle \otimes |y\rangle \\
|x\rangle \otimes (|y_1\rangle \otimes |y_2\rangle) &= |x\rangle \otimes |y_1\rangle + |x\rangle \otimes |y_2\rangle \\
c(|x\rangle \otimes |y\rangle) &= c|x\rangle \otimes |y\rangle = |x\rangle \otimes c|y\rangle
\end{aligned}$$

Suppose we have two vector spaces $H_1 = H_2 = \text{span}\{|0\rangle, |1\rangle\}$ over $\mathbb{C}$. Let the orthonormal basis for both H_1 and H_2 be $\text{span}\{|0\rangle, |1\rangle\}$. If $|\psi_1\rangle = |0\rangle + |1\rangle \in H_1$ and $|\psi_2\rangle = -|0\rangle + 2|1\rangle \in H_2$ then $|\psi_1\rangle \otimes |\psi_2\rangle = (|0\rangle + |1\rangle) \otimes (-|0\rangle + 2|1\rangle) = -|0\rangle \otimes |0\rangle + 2|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle + 2|1\rangle \otimes |1\rangle$. Moreover, $H_1 \otimes H_2$ is a tensor product space with basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Here we are denoting $|a\rangle \otimes |b\rangle$ by $|ab\rangle$.

Now we will see how do the operators act on a tensor product space. If $S : X \to V$ and

$T : Y \to W$ are two linear maps then the tensor product of S and T is a linear map

$$S \otimes T : X \otimes Y \to V \otimes W$$

defined by

$$(S \otimes T)(x \otimes y) = S(x) \otimes T(y)$$

Suppose S is an inverter, i.e. S changes a qubit from $|0\rangle$ to $|1\rangle$ and from $|1\rangle$ to $|0\rangle$. Mathematically, $S|0\rangle = |1\rangle$ and $S|1\rangle = |0\rangle$. Let the operator T be defined by $T|0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$, $T|1\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle$. The operator T is called the Hadamard operator. Then

$$(S \otimes T)(|0\rangle \otimes |1\rangle) = S|0\rangle \otimes T|1\rangle = |1\rangle \otimes \left(\frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle\right) = \frac{1}{\sqrt{2}}|10\rangle - \frac{1}{\sqrt{2}}|11\rangle$$

In quantum computers, an operator is implemented by quantum gates. Putting two quantum gates in series is equivalent to the application of the product of two operators on a tensor. We can simplify the product of two operators by the following way. If $(P \otimes Q)(S \otimes T)$ acts on a tensor $|a\rangle \otimes |b\rangle$ then we get,

$$(P \otimes Q)(S \otimes T)(|a\rangle \otimes |b\rangle) = (P \otimes Q)(S(|a\rangle) \otimes T(|a\rangle)) = PS(|a\rangle) \otimes QT(|a\rangle) = (PS \otimes QS)(|a\rangle \otimes |a\rangle)$$

Therefore, $(P \otimes Q)(S \otimes T) = PS \otimes QT$ We can generalize it and get the following.

$$(A_1 \otimes A_2 \otimes \cdots A_n)(B_1 \otimes B_2 \otimes \cdots B_n) = A_1B_1 \otimes A_2B_2 \otimes \cdots A_nB_n$$

The matrix representation of the tensor product of two operators can be obtained by the Kronecker product of the matrices of corresponding two operators under a standard choice of bases of the tensor products. This fact will be explained by the following example.

Let us define operators S and T on the Hilbert spaces $H_1 = \text{span}\{|0\rangle, |1\rangle\}$ and $H_2 = \text{span}\{|0\rangle, |1\rangle\}$ by

$$\begin{aligned} T|0\rangle &= |0\rangle - i|1\rangle; \quad T|1\rangle = i|0\rangle + |1\rangle \\ S|0\rangle &= i|1\rangle; \quad S|1\rangle = -i|0\rangle \end{aligned}$$

Then,

$$\begin{aligned} (S\otimes T)(2|01\rangle - |10\rangle) &= 2S|0\rangle T|1\rangle - S|1\rangle T|0\rangle \\ &= 2i|1\rangle(i|0\rangle + |1\rangle) - S|1\rangle T|0\rangle \\ &= i|1\rangle(i|0\rangle + |1\rangle) - i|0\rangle(|0\rangle - i|1\rangle) \\ &= i|00\rangle + |01\rangle - 2|10\rangle + 2i|11\rangle \end{aligned}$$

The matrix representations for S, T and the Kroncker product of S and T (also denoted by $S\otimes T$) are the following. $S = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $T = \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$ and

$$S\otimes T = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & i & 1 \\ 0 & 0 & -1 & -i \\ i & -1 & 0 & 0 \\ 1 & i & 0 & 0 \end{pmatrix}$$

Therefore,

$$(S\otimes T)(2|01\rangle - |10\rangle = \begin{pmatrix} 0 & 0 & i & 1 \\ 0 & 0 & -1 & -i \\ i & -1 & 0 & 0 \\ 1 & i & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 2 \\ -1 \\ 0 \end{pmatrix} = \begin{pmatrix} i \\ 1 \\ -2 \\ 2i \end{pmatrix} = i|00\rangle + |01\rangle - 2|10\rangle + 2i|11\rangle$$

If $|x\rangle \otimes |y\rangle$ is a tensor in a tensor product space then

$$\begin{aligned} \alpha(A\otimes B)(|x\rangle \otimes |y\rangle) &= \alpha(A|x\rangle \otimes B|y\rangle) \\ &= (\alpha A|x\rangle) \otimes B|y\rangle \\ &= A|x\rangle \otimes (\alpha B)|y\rangle \end{aligned}$$

Therefore, for any operators A, B and a scalar α we have $\alpha(A\otimes B) = (\alpha A)\otimes B = A\otimes(\alpha B)$.

Remark II.2.1. *If $T = A\otimes B$ is an operator on a finite dimensional Hilbert space then we can write*

$$T = JC\otimes D$$

where $J \geq ||A||\cdot||B||$ and $||C||, ||D|| \leq 1$. This is true for the following reason. Choose $J_1 \geq ||A||$ and $J_2 \geq ||B||$. Let $C = \frac{1}{J_1}A$, $D = \frac{1}{J_2}B$, and $J = J_1 J_2$. Then $T = J\left(\frac{1}{J_1}A\right)\otimes\left(\frac{1}{J_2}B\right) = JC\otimes D$. We can easily extend it for $T = A_1\otimes A_2\otimes\cdots\otimes A_n$.

Remark II.2.2. *Let $T = A_1\otimes A_2\otimes A_3\otimes\cdots A_n + B_1\otimes B_2\otimes\cdots\otimes B_m$ where A_i, and B_j's are operators on a finite dimensional Hilbert spaces. Then we can write,*

$$T = J(C_1\otimes C_2\otimes C_3\otimes\cdots C_n + D_1\otimes D_2\otimes\cdots\otimes D_m)$$

where $||C_1||, ||C_2||, \cdots, ||C_n|| \leq 1$ *and* $||D_1||, ||D_2||, \cdots, ||D_m|| \leq 1$

Using Remark (II.2.1) we can find J_A *and* J_B *such that*

$$T = J_A(C'_1 \otimes C_2 \otimes C_3 \otimes \cdots C_n) + J_B(D'_1 \otimes D_2 \otimes \cdots \otimes D_m)$$

where $||C'_1||, ||D'_1|| \leq 1$ *and* $||C_i||, ||D_j|| \leq 1$ *for all* $i > 1$ *and* $j > 1$. *Now take* $J = \max\{J_A, J_B\}$. *Then*

$$\begin{aligned} T &= J\left(\frac{J_A}{J}C'_1\right) \otimes C_2 \otimes C_3 \otimes \cdots C_n + J\left(\frac{J_B}{J}D'_1\right) \otimes D_2 \otimes \cdots \otimes D_m \\ &= JC_1 \otimes C_2 \otimes C_3 \otimes \cdots C_n + JD_1 \otimes D_2 \otimes \cdots \otimes D_m \end{aligned}$$

where $||C_1||, ||C_2||, \cdots, ||C_n|| \leq 1$ *and* $||D_1||, ||D_2||, \cdots, ||D_m|| \leq 1$

Remark (II.2.1) and remark (II.2.2) are important for our work because we will find an effective Hamiltonians for a target Hamiltonian of form $H_{\text{target}} = JA \otimes B$ and $H_{\text{target}} = JA \otimes B \otimes C$ where $||A||, ||B||, ||C|| \leq 1$ and J is a constant. If the norms of A, B, C are not bounded by 1 then we can use these two remarks to rewrite H_{target} in an equivalent form to find an effective Hamiltonian. Now we will formally discuss about bits, qubits and quantum algorithm.

Bits and 1-Qubit System

Bit is the basic unit which is used to store information in conventional computer. Each bit can store only two possible values, 0 or 1. To store an integer number, we represent it in binary and then we store it in the memory of a computer. For example the binary representation of 9 is 1001, and so we need at least 4 bits to store this number. To store an English letter or any other character, i.e '@', '#', '%' etc, we encode the character in binary. We use a block of eight bits to store the encoded character. A block of eight bits is called a byte.

Quantum computer uses the principle of quantum mechanics. Superposition and entanglement are two phenomenon which are present in quantum computers but not in the traditional computers. **Qubit** is the quantum analog of bit. A qubit has two stationary states represented by $|0\rangle$ and $|1\rangle$ which are equivalent to 0 and 1 respectively. A qubit can also be in superposition state which is a linear combination of these two states. When we measure a qubit, there is a probability p that the outcome would be $|0\rangle$ and there is a probability $1-p$ that the outcome would be $|1\rangle$. If a qubit is in state $\frac{3}{5}|0\rangle+\frac{4}{5}|1\rangle$ then the probability that the outcome of a measurement would be $|0\rangle$ and $|1\rangle$ are $\frac{9}{25}$ and $\frac{16}{25}$ respectively. If a qubit is in $|0\rangle$ state then the probability of getting $|0\rangle$ is 1 and the probability of getting $|1\rangle$ is 0.

n-Qubit System

A n-qubit system consists of n qubits and the possible states of this system come from the tensor product space $H^{\otimes n} = H \otimes H \otimes \cdots$ (n times), where $H = \text{span}\{|0\rangle, |1\rangle\}$ over $\mathbb{C}$. The system can have two types of states: pure state, and entangled state. If the states of n qubits are $|i_1\rangle, |i_2\rangle, \cdots |i_n\rangle$ then the state of the system is

$$|i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle$$

This state is called a pure state. In other words, if a state of the system can be expressed in this form then it is called pure state. Otherwise it is called entangled state. More specifically, a state $|\psi\rangle$ in a tensor product space $H_1 \otimes H_2$ is called an entangled state if it cannot be written as a tensor product $|\psi_1\rangle \otimes |\psi_2\rangle$ where $|\psi_1\rangle \in H_1$ and $|\psi_2\rangle \in H_2$.

Example II.2.1. *Suppose the states of qubits in a 2-qubit system are* $i_1 = \frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle$ *and* $i_2 = \frac{12}{13}|0\rangle + \frac{5}{13}|1\rangle$. *Then the state of the system is* $|i_1\rangle \otimes |i_2\rangle$, *which can also be written as* $|i_1 i_2\rangle$

where

$$|i_1 i_2\rangle = |i_1\rangle \otimes |i_2\rangle = \left(\frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle\right)\left(\frac{12}{13}|0\rangle + \frac{5}{13}|1\rangle\right) = \frac{36}{65}|00\rangle + \frac{15}{65}|01\rangle + \frac{48}{65}|10\rangle + \frac{20}{65}|11\rangle$$

The state $\frac{36}{65}|00\rangle + \frac{15}{65}|01\rangle + \frac{48}{65}|10\rangle + \frac{20}{65}|11\rangle$ *is a pure state. It is also a superposed state because it is a linear combination of four stationary states* $|00\rangle, |01\rangle, |10\rangle, |11\rangle$

Example II.2.2. *Suppose the states of* 4 *qubits are* $i_1 = i_2 = \frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle$ *and* $i_3 = i_4 = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$. *The state of the system is* $|i_1\rangle \otimes |i_2\rangle \otimes |i_3\rangle \otimes |i_4\rangle$ *which can be written as* $|i_1 i_2 i_3 i_4\rangle$, *i.e.*

$$|i_1 i_2 i_3 i_4\rangle = |i_1\rangle \otimes |i_2\rangle \otimes |i_3\rangle \otimes |i_4\rangle = \sum C_i |abcd\rangle$$

where $a, b, c, d = 0$ *or* 1. *This is another example of pure state.*

Example II.2.3. *Suppose a* 2*-qubit system is in the state* $\psi = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. *We can easily show that this is an entangled state. If* $\psi = (a_1|0\rangle + b_1|1\rangle) \otimes (a_2|0\rangle + b_2|1\rangle)$ *then* $\psi = a_1a_2|00\rangle + b_1a_2|10\rangle + a_1b_2|01\rangle + b_1b_2|11\rangle$. *This implies that* $a_1a_2 = 0$. *Hence either* $a_1 = 0$ *or* $a_2 = 0$. *But if* $a_1 = 0$ *then the coefficient of* $|01\rangle$ *is* 0, *which is a contradiction. If* $a_2 = 0$ *then the coefficient of* $|10\rangle$ *is* 0, *which is again a contradiction. Therefore* ψ *cannot be written as* $|i_1\rangle \otimes |i_2\rangle$ *and so* ψ *is an entangled state.*

Both superposed states and entangled states are very important in quantum computation. In Shor's factoring algorithm, entanglement enables the algorithm runs efficiently. Entanglement is used in quantum information theory to send two classical bits using only one qubit. This technique is called superdense coding. Quantum teleportation, also called entanglement-assisted teleportation, is a technique that can transmit a qubit from one location to another without the qubit being transmitted through the intervening space. In this technique, the receiver and sender share a maximally entangled state beforehand [1]. Entangled photon is used in quantum cryptography where highly secure keys were established using polarizing entangled photon pairs [6]. A superposed state of a system of n qubits simultaneously stores all the numbers from 0 to $2^n - 1$. For example, a 4-qubit system can store numbers from 0 to 15 with different probabilities. If $i_1 = i_2 = \frac{3}{5}|0\rangle + \frac{4}{5}|1\rangle$, $i_3 = i_4 = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$ then the probability that the outcome of a measurement will be $|0000\rangle$, $|0101\rangle$, and $|1111\rangle$ are $\left(\frac{3}{5}\right)^2\left(\frac{3}{5}\right)^2\left(\frac{1}{\sqrt{2}}\right)^2\left(\frac{1}{\sqrt{2}}\right)^2 = \frac{81}{2500}$, $\left(\frac{3}{5}\right)^2\left(\frac{4}{5}\right)^2\left(\frac{1}{\sqrt{2}}\right)^2\left(\frac{1}{\sqrt{2}}\right)^2 = \frac{144}{2500}$ and $\left(\frac{4}{5}\right)^2\left(\frac{4}{5}\right)^2\left(\frac{1}{\sqrt{2}}\right)^2\left(\frac{1}{\sqrt{2}}\right)^2 = \frac{256}{2500}$ respectively. A traditional computer cannot store more than one number simultaneously.

II.2.2 Quantum Algorithm

To understand the basic idea for quantum algorithm, we need to know the fundamental differences between the classical computers and quantum computers. In classical computers, n bits cannot store more than one number simultaneously. But in quantum computers, n qubits can store all the numbers from 0 to $2^n - 1$ simultaneously. If each number is equally probable then the probability of measuring any specific number is 2^{-n}. Another basic difference is that in classical computers we can read off the stored data as many times as we want without changing the stored value. But if we read off stored data in n-qubits of a quantum computer, which are in superposition state, then the superposition will be destroyed. Therefore, though all 2^n numbers are stored, only one number can be measured. This is the philosophy for quantum computation. The main idea for quantum algorithm is to do operation on stored data to increase the probability for getting useful result during measurement. In quantum computation, by "operation on qubits" we mean the application of unitary transformation on qubits.

Example II.2.4. *Suppose a 2-qubit system is in pure state $|i_1 i_2\rangle = |i_1\rangle \otimes |i_2\rangle$ where $|i_1\rangle =$*

$|i_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Then

$$|i_1 i_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{2}|00\rangle + \frac{1}{2}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{2}|11\rangle$$

The outcome of a measurement will be $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ with probability $\frac{1}{4}$. Let

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

Multiplying the state $|i_1 i_2\rangle$ by U we get,

$$U|i_1 i_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(-|00\rangle + |11\rangle)$$

We get a new superposition state $\frac{1}{\sqrt{2}}(-|00\rangle + |11\rangle)$. This state is an entangled state. After applying U on $|i_1 i_2\rangle$ the probability that the outcome of a measurement will be $|00\rangle, |01\rangle, |10\rangle$ and $|11\rangle$ becomes $\frac{1}{2}$, 0, 0 and $\frac{1}{2}$ respectively.

II.2.3 Quantum Gates

Quantum gates are the basic building blocks for quantum computers. They are used to manipulate data which are stored in memory. All quantum gates are reversible, because they are unitary operations. The logic gates for classical computers are not reversible. For example, the AND gate has four possible input combinations and two possible outputs. Four inputs cannot map to two outputs with an invertible operation. Therefore AND gate is not reversible. We will discuss some very important gates, which are used in quantum computers.

1-qubit Gate

Let us start with NOT gate (inverter). It has one input an one output. If we represent this operation by operator X, then by applying X on state $|i\rangle = \alpha|0\rangle + \beta|1\rangle$ we must get,

$$X|i\rangle = X(\alpha|0\rangle + \beta|1\rangle) = \beta|0\rangle + \alpha|1\rangle$$

To find the matrix representation of X, we will apply it on the basis vectors $|0\rangle$ and $|1\rangle$.

$$\begin{aligned} X|0\rangle &= X(1|0\rangle + 0|1\rangle) = 0|0\rangle + 1|1\rangle = |1\rangle \\ X|1\rangle &= X(0|0\rangle + |1\rangle) = 1|0\rangle + 0|1\rangle = |0\rangle \end{aligned}$$

Therefore, the matrix representation of X is $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

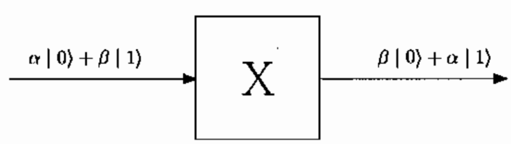


Figure II.1. Quantum Inverter

Hadamard gate is a very useful gate used in quantum computers. If R represents the operator for Hadamard gate then R is defined as follows.

$$\begin{aligned} R|0\rangle &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ R|1\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{aligned}$$

Therefore, the matrix representation for R is

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

If the state of a qubit is $|0\rangle$ then Hadamard gate changes the probability of getting $|0\rangle$ to $\frac{1}{2}$.

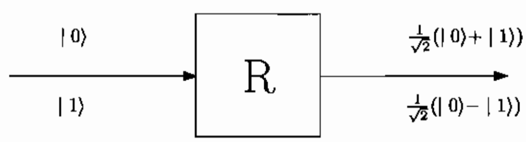


Figure II.2. Hadamard Gate

Pauli-X, Pauli-Y and Pauli-Z gates are represented by

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The following is the matrix representation of Phase shift gates.

$$R_\theta = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

If $\theta = \pi$, $\frac{\pi}{2}$, and $\frac{\pi}{4}$ then we get Pauli-Z gate, phase gate and $\frac{\pi}{8}$ gate, respectively. Now we will see some gates which operate on two qubits.

2-qubit Gate

Swap gate swaps two qubits. Hence the swap operator S operators on $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ and gives the following outputs.

$$S|00\rangle = |00\rangle, \qquad S|01\rangle = |10\rangle, \qquad S|10\rangle = |01\rangle, \qquad S|11\rangle = |11\rangle$$

Therefore the matrix for S is

$$S = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Controlled gates contain an extra bit called control bit which controls the output. Controlled NOT gate has two inputs, one of which is the control bit. If the control qubit is 0 then the other qubit does not change. If the control qubit is 1 then the other qubit is inverted.

$$CNOT|00\rangle = |00\rangle, \qquad CNOT|01\rangle = |01\rangle, \qquad CNOT|10\rangle = |11\rangle, \qquad CNOT|11\rangle = |10\rangle$$

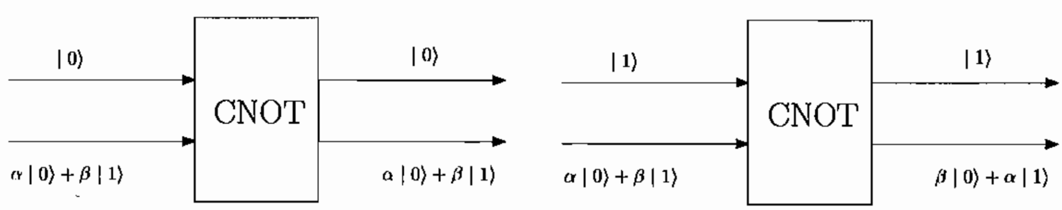


Figure II.3. Controlled NOT gate

We can generalize this gate to construct a controlled U gate. Let the operator U be the following.

$$U = \begin{pmatrix} \alpha_{00} & \alpha_{01} \\ \alpha_{10} & \alpha_{11} \end{pmatrix}$$

The controlled U gate maps the basis vectors in the following way.

$$\begin{aligned} CU|00\rangle &= |00\rangle, \qquad CU|01\rangle = |01\rangle \\ CU|10\rangle &= |1(\alpha_{00}|0\rangle + \alpha_{01}|1\rangle)\rangle \\ CU|11\rangle &= |1(\alpha_{10}|0\rangle + \alpha_{11}|1\rangle)\rangle \end{aligned}$$

The matrix for this gate is $CU = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \alpha_{00} & \alpha_{01} \\ 0 & 0 & \alpha_{10} & \alpha_{11} \end{pmatrix}$

3-qubit Gate

The gates in classical computers do not perform reversible operation. A 2-bit AND gate or 2-bit OR gate has four possible inputs (00, 01, 10, 11) but only two outputs (0,1). Four inputs cannot map reversibly to two outputs which makes these gates irreversible. We cannot even make them reversible by adding one extra bit at the output. The reason is the following. Suppose we have two output bits and the first bit gives the output and the second bit is the extra bit called ancillary bit. Then for AND gate, three inputs (00, 01 and 10) must map to the output whose first bit is 0. But we have only two outputs with first bit 0 (00, 01). For OR gate, three inputs (01, 10 and 11) must map to the output whose first bit is 1. But we have only two outputs with first bit 1. (10, 11). This shows that, by adding one extra bit at the output we cannot construct a reversible AND gate or OR gate. For constructing reversible AND or OR gate we need an extra input bit. We will call these extra bit ancilla.

Toffoli gate is a reversible gate with 3 inputs and 3 outputs. Toffoli proposed this gate in 1980. Using Toffoli gate we can implement classical AND gate and NOT gate. Since any boolean function can be implemented by these two gates, we can implement any classical logic circuit using Toffoli gate. The truth table for Toffoli gate is the following. This mapping can

Table II.1. Truth table for Toffoli gate

Inputs			Outputs		
a	b	c	x	y	z
0	0	0	0	0	0
0	0	1	0	0	1
0	1	0	0	1	0
0	1	1	0	1	1
1	0	0	1	0	0
1	0	1	1	0	1
1	1	0	1	1	1
1	1	1	1	1	0

be described as $|a,b,c\rangle \rightarrow |a,b,(c \oplus ab)\rangle$ where $\oplus$ represents XOR. If $c = 0$ then $|a,b,0\rangle \rightarrow |a,b,(ab)\rangle$. So if we consider a and b are our inputs then $z = ab$ gives the output which is equivalent to AND operation. If $a = b = 1$ then $|1,1,c\rangle \rightarrow |1,1(c \oplus 11)\rangle = |1,1(NOTc)\rangle$. This is the NOT operation for input c.

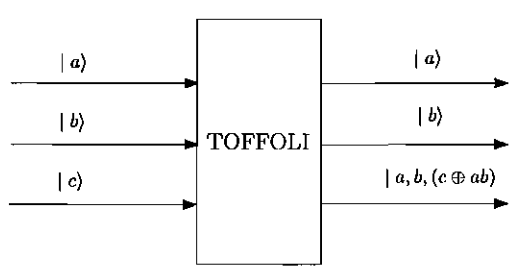


Figure II.4. Toffoli Gate

CHAPTER III

EFFECTIVE HAMILTONIAN FOR SYSTEM OF BOSONS OR FERMIONS

"The many-body problem is the study of the effects of interactions between particles on the behavior of a many-particle system"([10]). Many-body problem appears in quantum mechanics to solve the system that contains more than one particle. In general a many-body system with many particle interactions is almost impossible to solve. The main difficulty comes from the interaction terms in the Hamiltonian. For a magnetically ordered crystal near the ground state, the exact Hamiltonian can be approximated by Heisenberg Hamiltonian which is a sum of exchange Hamiltonians for all pairs of atoms. Hence the complicated total Hamiltonian can be replaced by a simple 2-body Heisenberg Hamiltonian. In quantum computation, a k-body Hamiltonian acting on n qubits can be approximated by a 2-body Hamiltonian. We want to find an approximate 2-body effective Hamiltonian to replace the exact Hamiltonian of a system of bosons or fermions.

III.1 Problem Description and Strategy

In the second quantization, the Hamiltonian of bosons and fermions are composed of creation operators and annihilation operators. These Hamiltonians can be rewritten as a sum of operators of form $JABC\cdots$ where J is a constant and each of $A,B,C,\cdots$ are of form $b_i^\dagger b_j$ or $a_i^\dagger a_j$. So $A,B,C\cdots$ can be viewed as one particle operators. We will find a 2-body effective Hamiltonian by decomposing $JABC\cdots$, such that the lowest eigenvalue of the effective Hamiltonian is ε-close to the lowest eigenvalue of the target Hamiltonian. Recall that a Hamiltonian $H=\sum H_i$ is called a k-body Hamiltonian if each H_i acts on no more than k particles.

The main idea for solving this problem is the following. If an operator is of form $A_1\cdot A_2\cdot A_3\cdots A_n$ then we will write $(A_1\cdot A_2\cdot A_3\cdots A_i)\cdot(A_{i+1}\cdots A_n)=AB$ where $A=A_1\cdot A_2\cdot A_3\cdots A_i$ and $B=A_{i+1}\cdots A_n$. Then we will decompose it to find an effective Hamiltonian $H_{\text{eff}}=H_1+H_2$

such that H_1 contains A but not B and H_2 contains B but not A. To decompose it we will use an extra particle with two states. The extra particle for decomposing the operators, will be called a subdivision gadget. We will apply this procedure several times to get a Hamiltonian that contains no more than three operators in each term. Then we will use another extra particle to decompose the terms which contains three operators. This extra particle will be called 3-to-2 gadget and this will give an effective Hamiltonian in the required form.

III.2 2-Body Effective Hamiltonian for k-Body Hamiltonian acing on n qubits

Construction of a 2-body effective Hamiltonian for a k-body Hamiltonian acting on n qubits is shown in [2]. The key idea to solve this problem comes from the following equation [13].

$$\begin{aligned} e^S He^{-S} &= \left(1+S+\frac{S^2}{2!}+\frac{S^3}{3!}+\cdots\right)H\left(1-S+\frac{S^2}{2!}-\frac{S^3}{3!}+\cdots\right) \\ &= H+(SH-HS)+\frac{1}{2!}(S^2H-2SHS+HS^2)+\cdots \\ &= H+[S,H]+\frac{1}{2}[S,[S,H]]+\frac{1}{3!}[S,[S,[S,H]]]+\cdots \end{aligned}$$

Therefore,

$$e^S He^{-S} = H+[S,H]+\frac{1}{2}[S,[S,H]]+\frac{1}{3!}[S,[S,[S,H]]]+\cdots \tag{III.1}$$

where S is an anti-Hermitian operator which makes $e^{\pm S}$ unitary. We take S of order of ε where ε is a small positive number. An operator is of order ε means that the operator norm of the operator is of order ε, and thus the operator norm goes to zero as ε goes to zero. If H is an operator of order ε^{-2} then $\frac{1}{3!}[S,[S,[S,H]]]$ and the following terms are all of order ε (see Lemma (III.2.2). So only first three terms will contribute to the effective Hamiltonian. If H is an operator of order ε^{-3} then $\frac{1}{4!}[S,[S,[S,[S,H]]]]$ and the following terms are all of order ε. For subdivision gadget we choose the effective Hamiltonian H or order ε^{-2} such that the first three terms of the series approximates the target Hamiltonian $H_{\text{target}} = JAB$. For 3-to-2 gadget we choose the effective Hamiltonian or order ε^{-3} such that first four terms approximates $H_{\text{target}} = JABC$. In the target Hamiltonian of form $H_{\text{target}} = JAB$ and $H_{\text{target}} = JABC$, J is a constant and $||A||, ||B|, ||C|| \leq 1$. Since for both subdivision gadget and 3-to-2 gadget first few terms approximate the target Hamiltonian and the rest of the terms of the series are of order ε, we can make them as small as we want by choosing appropriate ε. This is the main idea to find an effective Hamiltonian for a target Hamiltonian.

Since we are going to consider only the first few terms of equation (III.1), we need to know how fast is the tail of this series converging. We can show that the norm of the tail of the series (III.1) starting form the k-th term is bounded by a multiple of the norm of k-th term. The following lemma will mathematically explain an estimate of the tail. The proof for this lemma is given in appendix A.

Lemma III.2.1. *([2], p.3) Let S be an anti-Hermitian operator and X be an operator. Define a superoperator L such that $L(X) = [S,X]$ and $L^0(X) = X$. For any operator H and integer k define $r_k(H) = ||e^S He^{-S} - \sum_{p=0}^{k-1} L^p(H)||$ if $k \geq 1$ and $r_0(H) = ||e^S He^{-S}|| = ||H||$. Then for any $k \geq 1$ one has $r_k(H) \leq \frac{1}{k!}||L^k(H)||$.*

We also need to estimate the growth of $||L^k(H)||$. If S is an operator of $O(\varepsilon)$ and H is an operator of $O(\varepsilon^p)$ then $||L^k(H)|| = O(\varepsilon^{k+p})$. Formally this can be stated in the following way.

Lemma III.2.2. *([2], p.3) Let S and H be any $O(1)$-local operators acting on n qubits with $S = J_S A$ and $H = J_H B$ where J_S, J_H are constants and $||A||, ||B|| \leq 1$. Then for any $k = O(1)$ one has $||L^k(H)|| = O(J_S^k J_H)$*

The proof of this lemma is fairly straight forward and the proof will be given in Appendix A. Now we will present two gadgets called subdivision gadget and 3-to-2 gadget ([2], pp. 3-4). Subdivision gadget is used to decompose a target Hamiltonian of form $H_{\text{target}} = JAB$ where A

and B act on disjoint subset of qubits and 3-to-2 gadget is used to decompose a target Hamiltonian of form $H_{\text{target}} = JABC$ where A, B, and C act on different qubits and J is a constant. By "decompose" we mean to write the target Hamiltonian as a sum of operators which contain no more than one operator of A, B, and C. If an operator has the form $H = A_1A_2A_3\cdots A_n$ then we apply subdivision gadget repeatedly to get a sum of operators which contain no more than 3 operators. Then using 3-to-2 gadget we find a 2-body effective Hamiltonian. Therefore, combination of these two gadgets give a 2-body effective Hamiltonian for a k-body target Hamiltonian H_{target} acting on n qubits.

III.2.1 Subdivision Gadget([2], p.3)

If the exact Hamiltonian is of form $H_{\text{target}} = JAB$ where A, B act on non overlapping subsets of $\lceil k/2 \rceil$ or less qubits then we add an extra qubit called "Gadget" to decompose H_{target}. A gadget is simply a mediator qubit that mediates interaction between system qubits. Let us denote this qubit by u. We will define two projection operators for this qubit, $P_u = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ and $Q_u = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$. P_u is the projector onto low-energy subspace and Q_u is the projector onto high-energy subspace. The effective Hamiltonian H_{eff} for H_{target} is of form $H_{\text{eff}} = H_{u0} + V_u$ where $H_{u0} = \Delta Q_u$ and V_u is a perturbation. By choosing Δ sufficiently large we penalize the mediator qubit for being in $|1\rangle$ state and the proper choice of V^u will approximate H_{target} with an error of order ε. By choosing $S_u = -iJ^{1/2}(2\Delta)^{-1/2}\sigma_u \otimes (-A+B)$ and by applying Schrieffer-Wolff transformation e^{S_u}(equation III.1) on H_{eff} we transform H_{eff} into block diagonal form such that $P_u e^{S_u} H_{\text{eff}} e^{-S_u} Q_u = O(\varepsilon)$ and $P_u e^{S_u} H_{\text{eff}} e^{-S_u} P_u = H_{\text{target}} + O(\varepsilon)$.

By direct calculation and using Lemma III.2.1 and Lemma III.2.2 we can show that

$$\begin{aligned} e^{S_u} H_{\text{eff}} e^{-S_u} &= \left(H_{\text{eff}} + [S_u, H_{\text{eff}}] + \frac{1}{2}[S_u,[S_u,H_{\text{eff}}]] \right) + O(J^{3/2}\Delta^{-1/2}) \\ &= \begin{bmatrix} JAB & 0 \\ 0 & \Delta J + O(J) \end{bmatrix} + O(J^{3/2}\Delta^{-1/2}) \end{aligned}$$

If we use projector P_u and let $\Delta = J\varepsilon^{-2}$, then we observe that $P_u e^{S_u} H e^{-S_u} P_u$ is ε-close to $H_{\text{target}} = JAB$. Subdivision gadget can be formulated in the following lemma.

Lemma III.2.3. *([2], p.3)*

Let the target Hamiltonian be a single k-qubit interaction $H_{target} = JAB$ where A, B act on non overlapping subsets of $\lceil k/2 \rceil$ or less qubits and $||A||, ||B|| \leq 1$. Introduce one mediator qubit u, choose a parameter $\varepsilon \ll 1$ and define the effective Hamiltonian Hamiltonian $H_{eff} = H_0 + V$, with

$$\begin{aligned} H_0 &= \Delta Q_u \\ V &= \sqrt{\frac{\Delta J}{2}} \sigma_x^u \otimes (-A+B) + \frac{J}{2}(A^2+B^2) \end{aligned}$$

If we choose $\Delta = J\varepsilon^{-2}$, then $P_u e^{S_u} H e^{-S_u} P_u$ is ε-close to $H_{target} = JAB$, where $S_u = -i\frac{\varepsilon}{\sqrt{2}}\sigma_y^u \otimes (-A+B)$ and $P = |0\rangle\langle 0|$. In particular, by making ε arbitrarily small we can make the difference between the smallest eigenvalues of H_{eff} and H_{target} as small as we want.

III.2.2 3-to-2 Gadget([2], p.3)

By applying subdivision gadget several times on a Hamiltonian of form $H_{\text{target}} = A_1 A_2 \cdots A_n$ we get a 3-body effective Hamiltonian. We need another gadget called 3-to-2 gadget for transforming a 3-body Hamiltonian to a 2-body effective Hamiltonian. By using the similar idea for subdivision gadget we get the following lemma.

Lemma III.2.4. *([2], p.3)*

Let the target Hamiltonian be a single 3-body interaction, $H_{target} = JABC$ *where* A, B, C *are one-qubit operators acting on different qubits and* $||A||, ||B||, ||C|| \leq 1$. *Introduce one mediator qubit* u *and define the effective Hamiltonian* $H_{eff} = H_0 + V$, *with*

$$\begin{aligned} H_0 &= \Delta Q_u \\ V_d &= -\Delta^{2/3} J^{1/3} Q_u \otimes C \\ V_{od} &= \frac{\Delta^{2/3} J^{1/3}}{\sqrt{2}} \sigma_x^u \otimes (-A + B) \\ V_{extra} &= \Delta^{1/3} J^{2/3} (-A + B)^2 / 2 + J(A^2 + B^2) C / 2 \end{aligned}$$

If we choose $\Delta = J\varepsilon^{-3}$, *then* $P_u e^{S_u} H_{eff} e^{-S_u} P_u$ *is* ε*-close to* $H_{target} = JABC$ *where* $S_u = -\frac{i\varepsilon}{\sqrt{2}} \sigma_y^u \otimes R$, $R = (-A + B)\{I + \varepsilon C + \varepsilon^2 C^2 - \frac{2\varepsilon^2}{3} (-A + B)^2\}$ *and* $P = |0\rangle\langle 0|$. *In particular, by making* ε *arbitrarily small we can make the difference between the smallest eigenvalues of* H_{eff} *and* H_{target} *as small as we want.*

To apply subdivision gadget for the Hamiltonian of bosons or fermions we need to extend it for Hamiltonian of form $H_{\text{target}} = AB$ where A and B are non-commuting operators. We also need to show that the 3-to-2 gadget can be expanded for the case when A, B, C act on disjoint subspaces. We will explain these two extended gadgets in the following section.

III.3 Effective Hamiltonian for non-commuting operators

The requirement of commutativity of A and B in $H_{\text{target}} = JAB$ is an important drawback of subdivision gadget. If A and B are non-commuting operators, then we cannot apply this gadget to find an effective Hamiltonian. For example, the annihilation operators or creation operators of bosons or fermions do not commute. One of our main goals is to find a subdivision gadget which is applicable for non-commuting operators. In the following theorem we will give an effective Hamiltonian for the target Hamiltonian of form $H_{\text{target}} = \frac{J}{2}(AB+BA)$ where J is a constant and A, B are two operators.

Theorem III.3.1. *Let the target Hamiltonian be $H_{target} = \frac{J}{2}(AB+BA)$ where $||A||,||B|| \leq 1$. Introduce a two dimensional mediator Hilbert space $\mathcal{H} = span\{|0\rangle,|1\rangle\}$ over $\mathbb{C}$. If we define the effective Hamiltonian $H_{eff} = H_0 + V$, with*

$$
\begin{aligned}
H_0 &= J\varepsilon^{-2}Q_u \\
V &= V_1 + V_{extra} \\
V_1 &= \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u \otimes (-A+B) \\
V_{extra} &= (J/2)(A^2+B^2)
\end{aligned}
$$

then $P_u e^{S_u} H_{eff} e^{-S_u} P_u$ is close to $H_{target} = \frac{J}{2}(AB+BA)$ where $S_u = -i\frac{\varepsilon}{\sqrt{2}}\sigma_y^u \otimes (-A+B)$. Moreover the lowest eigenvalue of H_{target} is ε-close to the lowest eigenvalue of H_{eff}.

We used $\Delta = J\varepsilon^{-2}$ in Lemma (III.2.3) to get this subdivision gadget for non-commuting operators. The detail proof of this theorem is given in appendix B. Here we will give the sketch of the proof. For anti-Hermitian operator S_u we get (equation III.1),

$$e^{S_u} H_{\text{eff}} e^{-S_u} = H_{\text{eff}} + [S_u, H_{\text{eff}}] + \frac{1}{2}[S_u,[S_u,H_{\text{eff}}]] + \frac{1}{3!}[S_u,[S_u,[S_u,H_{\text{eff}}]]] + \cdots$$

We can easily see that $[S_u,[S_u,[S_u,H_{\text{eff}}]]], [S_u,[S_u,[S_u,[S_u,H_{\text{eff}}]]]], \cdots$ are all $O(\varepsilon)$. Hence we only need to compute $[S_u,H]$, and $[S_u,[S_u,H_{\text{eff}}]]$. After detailed calculations we get

$$\begin{aligned}
[S_u,H_{\text{eff}}] &= -\frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u\otimes(-A+B)-J\sigma_z^u\otimes(-A+B)^2+O(J\varepsilon)\\
[S_u,[S_u,H_{\text{eff}}]] &= J\sigma_z^u\otimes(-A+B)^2-\sqrt{2}J\varepsilon\sigma_x^u\otimes(-A+B)^3+O(J\varepsilon^2)
\end{aligned}$$

Therefore,

$$\begin{aligned}
e^{S_u}H_{\text{eff}}e^{-S_u} &= H_{\text{eff}}+[S_u,H_{\text{eff}}]+\frac{1}{2}[S_u,[S_u,H_{\text{eff}}]]+\frac{1}{3!}[S_u,[S_u,[S_u,H_{\text{eff}}]]]+\cdots\\
&= J\varepsilon^{-2}Q_u+(J/2)(A^2+B^2)-\frac{J}{2}\sigma_z^u\otimes(-A+B)^2-\frac{\sqrt{2}J\varepsilon}{3}\sigma_x^u\otimes(-A+B)^3+\cdots\\
&= J\varepsilon^{-2}\begin{pmatrix}0&0\\0&1\end{pmatrix}+(J/2)\begin{pmatrix}1&0\\0&1\end{pmatrix}\otimes(A^2+B^2)-\frac{J}{2}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\otimes(-A+B)^2-O(J\varepsilon)+\cdots\\
&= \begin{pmatrix}\frac{J}{2}(AB+BA)&0\\0&J\varepsilon^{-2}I+J(A^2+B^2-(AB+BA)/2)\end{pmatrix}-O(J\varepsilon)+\cdots\\
&= \begin{pmatrix}\frac{J}{2}(AB+BA)&0\\0&J\varepsilon^{-2}I+O(J)\end{pmatrix}-O(J\varepsilon)+\cdots
\end{aligned}$$

Therefore, $P_u e^{S_u}H_{\text{eff}}e^{-S_u}P_u$ is close to $H_{\text{target}}=\frac{J}{2}(AB+BA)$.

This theorem is an extension of the lemma about subdivision gadget for the operators that act on different qubits (Lemma III.2.3). We can also use it for the operators that act on non-overlapping subspaces. If A and B act on different qubits or if they act on non overlapping Hilbert spaces then A and B commute. In that case H_{eff} is ε close to $H_{\text{target}}=\frac{J}{2}(AB+BA)=\frac{J}{2}(AB+AB)=JAB$. This agrees with the result about the effective Hamiltonian for commuting operators [2].

III.3.1 A numerical example that supports Theorem III.3.1

We used Maple to compute eigenvalues of $H_{\text{target}} = \frac{1}{2}(AB + BA)$ and eigenvalues of the effective Hamiltonian H_{eff} for different values of ε and for the following pair of A and B.

$$\text{pair1 } :A = \begin{bmatrix} 0.6 & 0.3 \\ 0.4 & 0.5 \end{bmatrix}; B = \begin{bmatrix} 0.42 & 0.65 \\ 0.18 & 0.54 \end{bmatrix}$$

$$\text{pair2 } :A = \begin{bmatrix} 0.1 & 0.5 \\ 0.4 & 0.1 \end{bmatrix}; B = \begin{bmatrix} 0.2 & 0.5 \\ 0.1 & 0.4 \end{bmatrix}$$

$$\text{pair3 } :A = \begin{bmatrix} 4 & 8 & 1 \\ 2.4 & 3.1 & 2 \\ 4.4 & 3.6 & 7.1 \end{bmatrix}; B = \begin{bmatrix} 0.31 & .375 & 0.33 \\ 0.105 & 2.2 & 0.27 \\ 0.38 & 0.444 & 0.36 \end{bmatrix}$$

$$\text{pair4 } :A = \begin{bmatrix} 0.2 & 0.4 & 0.05 & 0.35 \\ 0.12 & 0.155 & 0.1 & 0.1 \\ 0.02 & 0.18 & 0.405 & 0.3 \\ 0.05 & 0.1 & 0.15 & 0.2 \end{bmatrix}; B = \begin{bmatrix} 0.062 & 0.075 & 0.066 & 0.065 \\ 0.021 & 0.0.404 & 0.054 & 0.077 \\ 0.076 & 0.0888 & 0.072 & 0.089 \\ 0.012 & 0.023 & 0.034 & 0.045 \end{bmatrix};$$

We summarize our result in Table III.1. The last row of the table gives the exact eigenvalue of $\frac{1}{2}(AB + BA)$. The Maple code for this calculations is given in Appendix C.

Table III.1. Numerical computation that supports Theorem III.3.1

ε	Eigenvalue			
	pair1	pair2	pair3	pair4
1	0.04643601625	-0.006245493531	-0.01920163713	-0.01253876875
0.1	0.07491785698	-0.006562489632	-0.01900525826	-0.01716263543
0.01	0.07536567026	-0.006555021286	-.01899333754	-0.01722618572
0.001	0.07537017272	-0.006554945139	-0.01899321657	-0.01722682392
0.0001	0.07537021778	-0.006554946303	-0.01899586618	-0.01722691953
Exact	0.07537021817	-0.006554944214	-0.01899321532	-0.01722683031

Now we will restate the 3-to-2 gadget (Lemma III.2.4) for expanded subspaces. Though Lemma (III.2.4) is stated for the operators A,B,C which act on different qubits, we can expand it for the operators when A,B,C act on non-overlapping Hilbert spaces. We can do it because we only need the commutativity of A,B,C.

Theorem III.3.2. *Let the target Hamiltonian be $H_{target} = JABC$ where A, B and C act on non overlapping Hilbert spaces and $||A||,||B||,||C|| \leq 1$. Introduce a 2-dimensional mediator Hilbert space span$\{|0\rangle,|1\rangle\}$ over $\mathbb{C}$. If we define the effective Hamiltonian $H_{eff} = H_0 + V$, with*

$$\begin{aligned} H_0 &= J\varepsilon^{-3}Q_u \\ V_d &= -J\varepsilon^{-2}Q_u \otimes C \\ V_{od} &= J\frac{\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u \otimes (-A+B) \\ V_{extra} &= J\varepsilon^{-1}(-A+B)^2/2 + J(A^2+B^2)C/2 \end{aligned}$$

and $S_u = -\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R$ where $R = (-A+B)\{I+\varepsilon C+\varepsilon^2C^2 - \frac{2\varepsilon^2}{3}(-A+B)^2\}$ then $P_u e^{S_u} H_{eff} e^{-S_u} P_u$ is ε close to $H_{target} = JABC$. Moreover the lowest eigenvalue of H_{target} is ε-close to the lowest eigenvalue of H_{eff}.

We will give a very brief sketch of the proof. The detail proof is given in appendix B. From equation III.1 we get,

$$e^{S_u}H_{\text{eff}}e^{-S_u} = H_{\text{eff}} + [S_u, H_{\text{eff}}] + \frac{1}{2}[S_u,[S_u,H_{\text{eff}}]] + \frac{1}{3!}[S_u,[S_u,[S_u,H_{\text{eff}}]]] + \cdots$$

Now we only need to compute $[S_u,H_{\text{eff}}]$, $[S_u,[S_u,H_{\text{eff}}]]$, $[S_u,[S_u,[S_u,H_{\text{eff}}]]]$ using the fact that A and B commute since they are acting on non overlapping subspaces. Note that $[S_u,[S_u,[S_u,[S_u,H_{\text{eff}}]]]],\cdots$ are all $O(\varepsilon)$.

Using extensive calculations we get,

$$H_{\text{eff}}+[S_u,H_{\text{eff}}]+\frac{1}{2}[S_u,[S_u,H_{\text{eff}}]]+\frac{1}{3!}[S_u,[S_u,[S_u,H_{\text{eff}}]]]+\cdots=\begin{pmatrix} JABC & 0 \\ 0 & J\varepsilon^{-3}I+O(J\varepsilon^{-2}) \end{pmatrix}+O(J\varepsilon)$$

Therefore, $P_u e^{S_u} H_{\text{eff}} e^{-S_u} P_u$ is ε close to $H_{\text{target}} = JABC$ and the lowest eigenvalue of H_{eff} approaches to the lowest eigenvalue of $H_{\text{target}} = JABC$ as ε approaches to zero.

III.3.2 A numerical example that supports Theorem III.3.2

We used Maple to compute eigenvalues of $H_{\text{target}} = ABC$ and eigenvalues of the effective Hamiltonian H_{eff} for different values of ε and for the following sets of A, B and C.

$$\text{set1 } :A=\begin{bmatrix} 0.62 & 0.48 \\ 0.54 & 0.65 \end{bmatrix}; B=\begin{bmatrix} 2/7 & 576 \\ 1/7 & 4/7 \end{bmatrix}; C=\begin{bmatrix} 0.385 & 0.42 \\ 0.455 & 0.225 \end{bmatrix}$$

$$\text{set2 } :A=\begin{bmatrix} 0.2 & 0.4 & 0.05 \\ 0.12 & 0.155 & 0.1 \\ 0.22 & 0.18 & 0.355 \end{bmatrix}; B=\begin{bmatrix} 1/3 & 8/75 & 11/15 \\ 17/75 & 41/150 & 2/15 \\ 32/75 & 8/25 & 81/150 \end{bmatrix}; C=\begin{bmatrix} 0.05 & 0.1 & 0.15 \\ 0.2 & 0.25 & 0.3 \\ 0.35 & 0.4 & 0.45 \end{bmatrix}$$

We summarize our result in the Table III.2. The last row of the table gives the exact eigenvalue of ABC. The Maple code for this calculations is given in Appendix C. Like

Table III.2. Numerical computation that supports Theorem III.3.2

ε	Eigenvalue	
	set1	set2
1	-0.123028621379470	-0.0520986634855282
0.1	-0.124434694440622	-0.0242971186895731
0.01	-0.124722766342154	-0.0243341494855787
0.001	-0.124753216266981	-0.0243379414815374
0.0001	-0.124757132093037	-0.0246644776257028
Exact	-0.124756576223	-0.0243383443278075

the subdivision gadget for non-commutative operators, Theorem (III.3.2) is not easily extendable for the non-commuting operators. Our initial guess was that the effective Hamiltonian $H_{\text{eff}} = H_0 + V$ in Theorem (III.3.2) would be an effective Hamiltonian for $H_{\text{target}} = \frac{1}{6}(ABC + ACB + BAC + BCA + CAB + CBA)$ when A, B, C do not commute. But numerical computation shows that our intuition is not correct. We used $A = \begin{bmatrix} 0.2 & 0.4 \\ 0.4 & 0.6 \end{bmatrix}$, $B = \begin{bmatrix} 1/3 & 5/6 \\ 1/6 & 2/3 \end{bmatrix}$, $C = \begin{bmatrix} 0.35 & 0.4 \\ 0.45 & 0.2 \end{bmatrix}$ and found that the lowest eigenvalue of H_{eff} approaches to 0.0519829 though the exact eigenvalue of $\frac{1}{6}(ABC + ACB + BAC + BCA + CAB + CBA)$ is -0.00175979.

Suppose our target Hamiltonian is $H_{\text{target}} = \sum_u H^u_{\text{target}} + H_{\text{else}}$ where H_{else} are the additional terms that consist of only 2-body interactions and we will not treat these terms using gadgets. On the other hand, $H^1_{\text{target}} = A_1 A_2 \cdots A_n$, $H^2_{\text{target}} = B_1 B_2 \cdots B_m$ and so on are the terms in $\sum_u H^u_{\text{target}}$ and for each H^i_{target} we will apply different subdivision gadgets and 3-to-2 gadgets. The following theorem shows that the if we apply different subdivision gadgets and 3-to-2 gadgets for each term in $\sum_u H^u_{\text{target}}$ then the effective Hamiltonian constructed using this way is ε close to the target Hamiltonian H_{target} with respect to the ground state energy.

Theorem III.3.3. *Let $H_{target} = \sum_u H^u_{target} + H_{else}$ where H^u_{target}s are of form $\frac{J}{2}(AB + BA)$ or $JABC$. If $H = \sum_u H^u + H_{else}$, where H^u is the effective Hamiltonian for H^u_{target}, constructed using Theorem (III.3.1) and Theorem (III.3.2), then the ground state energy of H approximates the ground state energy of H_{target}.*

The proof for this theorem is given in appendix B.

III.3.3 Effective Hamiltonian for $H_{\text{target}} = JAB$ where $[A,B] = C$ and $||A||, ||B|| \leq 1$

We can rewrite the target Hamiltonian as follows.

$$H_{\text{target}} = JAB = \frac{J}{2}(AB+BA) + \frac{J}{2}[A,B] = \frac{J}{2}(AB+BA) + \frac{1}{2}JC = H_1 + H_2$$

where $H_1 = \frac{J}{2}(AB+BA)$ and $H_2 = \frac{1}{2}JC$. We can find an effective Hamiltonian for H_1 using Theorem III.3.1. If we add this effective Hamiltonian with H_2 then Theorem III.3.3 guarantees that the lowest eigenvalue of this operator approximates the lowest eigenvalue of target Hamiltonian H_{target}.

III.3.4 A numerical example that supports Theorem III.3.3

Consider the following sets of operators and the target Hamiltonians.

$$\text{set1 } : A = \begin{bmatrix} 0.6 & 0.3 \\ 0.4 & 0.5 \end{bmatrix}; B = \begin{bmatrix} 0.42 & 0.65 \\ 0.018 & 0.54 \end{bmatrix}$$

$$H_{\text{target}} = AB = \frac{1}{2}(AB+BA) + [A,B]$$

$$\text{set2 } : A = \begin{bmatrix} 0.6 & 0.3 \\ 0.4 & 0.5 \end{bmatrix}; B = \begin{bmatrix} 0.42 & 0.65 \\ 0.018 & 0.54 \end{bmatrix}; C = \begin{bmatrix} 0.5 & 0.2 \\ 0.1 & 0.4 \end{bmatrix}; D = \begin{bmatrix} 0.9 & 0.1 \\ 0.28 & 0.3 \end{bmatrix}$$

$$H_{\text{target}} = AB + CD = \frac{1}{2}(AB+BA) + [A,B] + \frac{1}{2}(CD+DC) + [C,D]$$

$$\text{set3 } : A = \begin{bmatrix} 0.2 & 0.4 & 0.05 \\ 0.12 & 0.155 & 0.1 \\ 0.22 & 0.18 & 0.355 \end{bmatrix}; B = \begin{bmatrix} 0.31 & 0.375 & 0.33 \\ 0.105 & 0.22 & 0.27 \\ 0.38 & 0.444 & 0.36 \end{bmatrix}$$

$$H_{\text{target}} = AB = \frac{1}{2}(AB+BA) + [A,B]$$

Computer generated values are given in the Table III.3. The last row of the table, gives the exact eigenvalue of H_{target}.

Table III.3. Numerical computation that supports Theorem III.3.3

ε	Eigenvalue		
	set1	set2	set3
1	0.0232439725126434	0.200529412704801	-0.0298213123602373
0.1	0.0522257495519369	0.222007509982134	-0.0301101844282670
0.01	0.0526942284232064	0.222422778118875	-0.0301068520439003
0.001	0.0526989407371730	0.222426968582667	-0.0301068176049739
0.0001	0.0526989847421646	0.222427007045220	-0.0301068276166916
Exact	0.0526989882712956	0.222427010938698	-0.0301068172370731

We are going to see some applications of Theorem III.3.1 and III.3.2. We will use these two theorems to construct an effective Hamiltonian for a system of bosons or fermions.

III.4 Effective Hamiltonian for a system of bosons

The annihilation operators or creation operators for bosons or fermions appear as a product in the second quantized form of Hamiltonian. We are interested in finding a 2-body effective boson Hamiltonian or fermion Hamiltonian for a system of bosons or fermions. To find the effective Hamiltonian for $H_{\text{target}} = JAB$, we assumed that the operator norm of A and B are bounded by 1. In general, the operator norm of $b_i b_j^\dagger$, and $b_i^\dagger b_j$ are not bounded by 1, but they are bounded by some constant J. If an operator is bounded by J then we can divide it by J to get a new operator which is bounded by 1. Then we can apply Theorem III.3.1 and Theorem III.3.2 to get the desired effective Hamiltonian. In this section, we will assume that all the operators are bounded by 1 for the sake of simplicity. We will give an algorithm to find an effective Hamiltonian for many boson system or many fermion system. First, we will give some examples to explain the main idea behind the algorithm.

III.4.1 Example1: effective Hamiltonian for $H_{\text{target}} = b_1^\dagger b_2^\dagger b_3^\dagger b_1 b_2 b_4$

For $b_1^\dagger$, there is at most one operator b_1 which does not commute with $b_1^\dagger$. Moreover, b_1 commutes with all other operators except $b_1^\dagger$. So we can bring $b_1^\dagger$ and b_1 together and rewrite the target Hamiltonian as $H_{\text{target}} = b_1^\dagger b_1 b_2^\dagger b_3^\dagger b_2 b_4$. We can repeat the procedure for $b_2^\dagger$ and b_2 and we get $H_{\text{target}} = (b_1^\dagger b_1)(b_2^\dagger b_2)(b_3^\dagger b_4) = ABC$ where $A = b_1^\dagger b_1$, $B = b_2^\dagger b_2$ and $C = b_3^\dagger b_4$. Since A, B and C commute, we can apply 3-to-2 gadget to find an effective Hamiltonian.

$$\begin{aligned} H_{\text{eff}} &= \varepsilon^{-3}Q_u - \varepsilon^{-2}Q_u \otimes C + \frac{\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u \otimes (-A+B) + \varepsilon^{-1}(-A+B)^2/2 + (A^2+B^2)C/2 \\ &\approx \varepsilon^{-3}Q_u - \varepsilon^{-2}Q_u \otimes C + \frac{\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u \otimes (-A+B) + \varepsilon^{-1}(-A+B)^2/2 \\ &= \varepsilon^{-3}Q_u - \varepsilon^{-2}Q_u \otimes b_3^\dagger b_4 + \frac{\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u \otimes (-b_1^\dagger b_1 + b_2^\dagger b_2) + \varepsilon^{-1}(-b_1^\dagger b_1 + b_2^\dagger b_2)^2/2 \end{aligned}$$

This is a 2-body boson Hamiltonian.

III.4.2 Example2: Effective Hamiltonian for $H_{\text{target}} = (b_1^\dagger b_2)(b_2^\dagger b_3)(b_4^\dagger b_5)$

Let $H_{\text{target}} = ABC$ where $A = b_1^\dagger b_2$, $B = b_2^\dagger b_3$ and $C = b_4^\dagger b_5$ where H_{target} is acting on a system of n bosons. Also let $H_1 = AB$. Since the operators A and B are linear operators on a finite dimensional vector space, they are bounded and so we can apply Theorem (III.3.1). Operators A and B don't commute but the commutator is

$$[A,B] = [b_1^\dagger b_2, b_2^\dagger b_3] = b_1^\dagger b_2 b_2^\dagger b_3 - b_2^\dagger b_3 b_1^\dagger b_2 = b_1^\dagger b_2 b_2^\dagger b_3 - b_1^\dagger (b_2 b_2^\dagger - 1) b_3 = b_1^\dagger b_3$$

Hence, $H_1 = AB = \frac{1}{2}(AB+BA) + \frac{1}{2}[A,B] = \frac{1}{2}(AB+BA) + \frac{1}{2}b_1^\dagger b_3$. Using Theorem III.3.1 we can find an effective Hamiltonian for $\frac{1}{2}(AB+BA)$. Therefore, the effective Hamiltonian H_{eff1} for the target Hamiltonian H_1 is

$$H_{\text{eff1}} \approx \varepsilon^{-2}Q_{u_1} + \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^{u_1} \otimes (-b_1^\dagger b_2 + b_2^\dagger b_3)$$

We multiply H_{eff1} by C and get

$$H_{\text{eff1}}C \approx \varepsilon^{-2}Q_{u_1}(b_3^\dagger b_4) - \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^{u_1}\otimes(b_1^\dagger b_2)(b_3^\dagger b_4) + \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^{u_1}\otimes(b_2^\dagger b_3)(b_3^\dagger b_4)$$

Now we apply 3-to-2 gadget for the second and the third term which will give us an effective 2-body Hamiltonian.

III.4.3 Example3: effective Hamiltonian for $H_{\text{target}} = (b_1^\dagger b_2)^2 b_2^\dagger b_3$

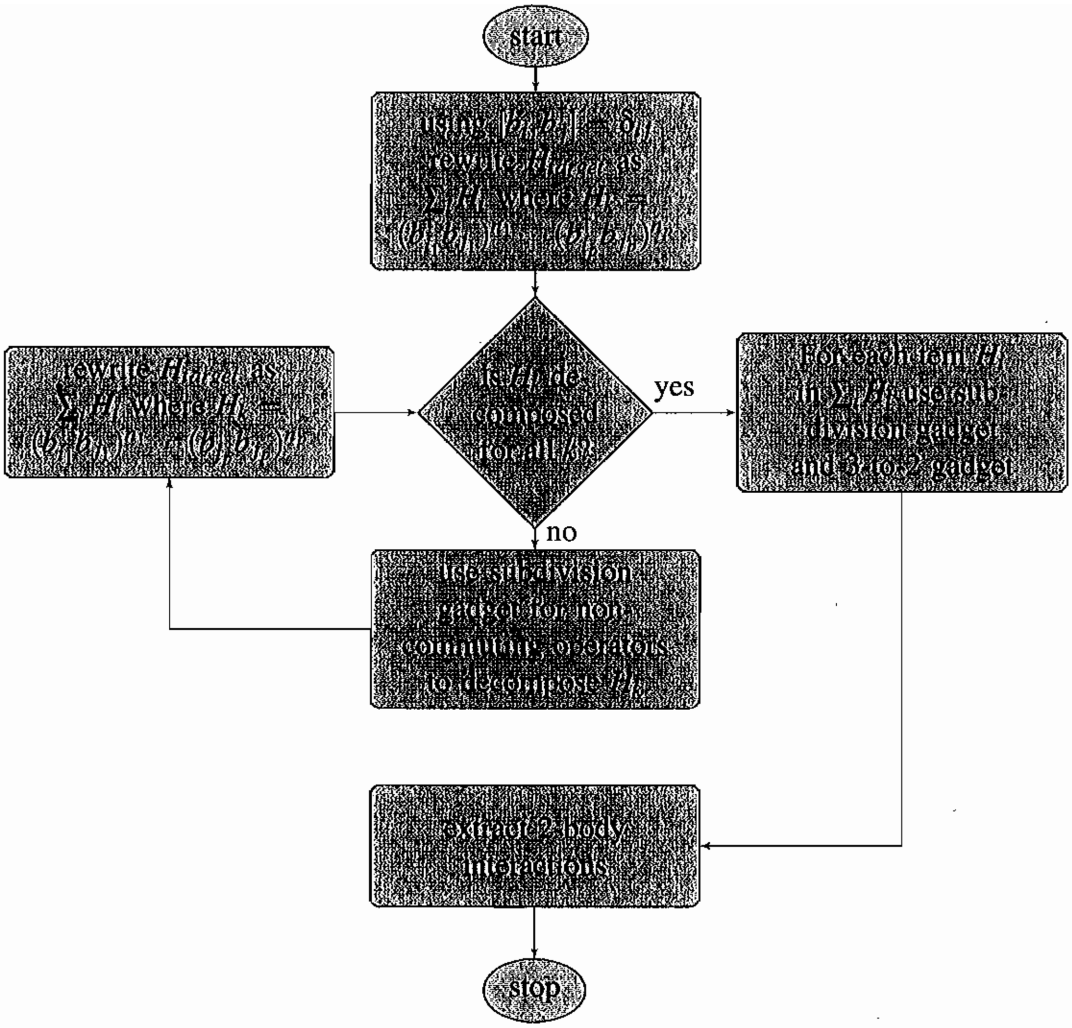
Let $H_{\text{target}} = A^2B$, where $A = (b_1^\dagger b_2)^2$ and $B = b_2^\dagger b_3$. The commutator $[A^2, B] = 2(b_1^\dagger b_2)(b_1^\dagger b_3)$. Applying subdivision gadget for non-commuting operators, we get

$$H_{\text{eff}} \approx \varepsilon^{-2}Q_u + \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u\otimes(-A^2+B) = \varepsilon^{-2}Q_u - \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u\otimes A^2 + \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u\otimes B$$

By applying 3-to-2 gadget for the second term, which contains $\sigma_x^u\otimes A^2$, we get a 2-body effective Hamiltonian.

III.4.4 An algorithm to find an effective Hamiltonian for $H_{\text{target}} = b_{k_1}^\dagger b_{k_2}^\dagger \cdots b_{k_n}^\dagger b_{p_1} b_{p_2} \cdots b_{p_n}$

Using the commutator $[b_i, b_j^\dagger] = \delta_{ij}$ we can bring $b_{k_1}^\dagger$ and b_{k_1} together and form a pair $(b_{k_1}^\dagger b_{k_1})$, if b_{k_1} is present in H_{target}. By repeating this process for all the operators we can rewrite H_{target} as $\sum_i H_k$ where $H_k = (b_{i_1}^\dagger b_{j_1})^{n_1}\cdots(b_{i_p}^\dagger b_{j_p})^{n_p}$. Let $A_k = (b_{i_k}^\dagger b_{j_k})^{n_k}$. Then $H_{\text{target}} = A_1A_2\cdots A_p$. Now for each term we apply subdivision gadget several times. Finally we apply 3-to-2 gadget to get an effective Hamiltonian. This procedure can be summarized by the following flowchart.



The many particle Hamiltonian in second quantization takes the form $H_{\text{target}} = H_1 + H_2 + H_3 + \cdots$. where H_i contains the annihilation and creation operators as a product. Using remark (II.2.2), we can write $H_{\text{target}} = J(A_1A_2\cdots A_{n_1} + B_1B_2\cdots B_{n_2} + \cdots)$ where $||A_i||, ||B_i|| \cdots \leq 1$ and J is a constant. Than we can find an effective Hamiltonian for H_{target} by applying the above algorithm.

III.5 Effective Hamiltonian for system of fermions

Algorithm for finding the effective Hamiltonian for the second quantized form of Hamiltonian of fermions is similar to the Hamiltonian of bosons. One of the main differences is the anti-commutation relation between $a_i^\dagger$ and a_i instead of commutation relation between $b_i^\dagger$ and b_i. Here we will show some examples to find an effective Hamiltonian for fermions. Note that since we always consider finite dimensional spaces, the operator norm of $a_i^\dagger a_j$ is always bounded.

III.5.1 An Example: effective Hamiltonian for $H_{\text{target}} = a_1^\dagger a_2^\dagger a_3^\dagger a_1 a_2 a_4$

For $a_1^\dagger$, there is at most one operator a_1 for which anti-commutator is non-zero. Moreover, a_1 anti-commutes with all other operators except $a_1^\dagger$. So we can bring $a_1^\dagger$ and a_1 together and rewrite the target Hamiltonian as $H_{\text{target}} = -a_1^\dagger a_2^\dagger a_1 a_3^\dagger a_2 a_4 = a_1^\dagger a_1 a_2^\dagger a_3^\dagger a_2 a_4$. We can repeat the procedure for $a_2^\dagger$ and a_2 and we get $H_{\text{target}} = -(a_1^\dagger a_1)(a_2^\dagger a_2)(a_3^\dagger a_4) = ABC$ where $A = a_1^\dagger a_1$, $B = a_2^\dagger a_2$ and $C = a_3^\dagger a_4$. We can easily check that A, B and C commute. We apply 3-to-2 gadget to find an effective Hamiltonian for H_{target}.

$$
\begin{aligned}
H_{\text{eff}} &= -\varepsilon^{-3} Q_u + \varepsilon^{-2} Q_u \otimes C - \frac{\varepsilon^{-2}}{\sqrt{2}} \sigma_x^u \otimes (-A+B) - \varepsilon^{-1}(-A+B)^2/2 - (A^2+B^2)C/2 \\
&\approx -\varepsilon^{-3} Q_u + \varepsilon^{-2} Q_u \otimes C - \frac{\varepsilon^{-2}}{\sqrt{2}} \sigma_x^u \otimes (-A+B) - \varepsilon^{-1}(-A+B)^2/2 \\
&= -\varepsilon^{-3} Q_u + \varepsilon^{-2} Q_u \otimes a_3^\dagger a_4 - \frac{\varepsilon^{-2}}{\sqrt{2}} \sigma_x^u \otimes (-a_1^\dagger a_1 + a_2^\dagger a_2) - \varepsilon^{-1}(-a_1^\dagger a_1 + a_2^\dagger a_2)^2/2
\end{aligned}
$$

An algorithm to find the effective Hamiltonian for a system of fermions is similar to the algorithm for finding an effective Hamiltonian for a system of bosons. Only difference is that when we rewritten the operators in the form $H_{\text{target}} = sA_1A_2 \cdots A_n$ then s could be positive or negative. Then applying subdivision gadget and 3-to-2 gadget we will get the required effective Hamiltonian.

To find the effective Hamiltonian we used some extra particles which has two stationary states. It is not know if we can find an effective Hamiltonian without those extra particles.

CHAPTER IV

CONCLUSIONS

In this thesis, we extended subdivision gadget for non-commuting operators [2]. The authors in [2] developed an effective Hamiltonian for a product of two operators which are acting on disjoint qubits. Commutativity is the main property, which is used in the proof. In this thesis we extended their lemma and applied it for the system of bosons or fermions.

- We extended the lemma about subdivision gadget (Lemma III.2.3) for non-commuting operators (Theorem III.3.1)
- We extended the lemma about 3-to-2 gadget (Lemma III.2.4) for non-overlapping subspaces (Theorem III.3.2)
- We applied these extended lemmas for the second quantized form of Hamiltonian of bosons and Hamiltonian of fermions. We write an effective Hamiltonian $H_{\text{eff}} = \sum_i H_i$ for a system of bosons or fermions such that H_{eff} is a 2-body Hamiltonian.

The following are some of the possible extensions of this thesis.

- We extended the subdivision gadget for non-commuting operators but we did not extend 3-to-2 gadget for non-commuting operators. We can use the extended 3-to-2 gadget to avoid repeated application of subdivision gadget for the Hamiltonian of from ABC.
- Though we can find an effective 2-body Hamiltonian, the procedure is not simple and we need lots of extra particles (gadgets). This changes the system and makes the calculations harder. Heisenberg Hamiltonian is a 2-body Hamiltonian which approximates the exact Hamiltoinian without changing the system. We may try to find some other way to find the effective Hamiltonian without any extra particle.

- We used Maple to find the lowest eigenvalue of the effective Hamiltonian. We observed that if we make ε too small then the effective Hamiltonian starts to diverge. We may need to do further research to find the range of ε for which we can get the reasonable results.

APPENDICES

APPENDIX A

PROOF OF IMPORTANT LEMMAS

Lemma III.2.1. *([2], p.3) Let S be an anti-Hermitian operator. Define a superoperator L such that $L(X) = [S,X]$ and $L^0(X) = X$. For any operator H and integer k define $r_k(H) = ||e^S He^{-S} - \sum_{p=0}^{k-1} L^p(H)||$ if $k \geq 1$ and $r_0(H) = ||e^S He^{-S}|| = ||H||$. Then for any $k \geq 1$ one has $r_k(H) \leq \frac{1}{k!}||L^k(H)||$.*

Proof. Let $t \geq 0$. Define $H(t) = e^{St}He^{-St}$ and

$$r_k(H,t) = \left|\left| H(t) - \sum_{p=0}^{k-1} \frac{t^p}{p!} L^p(H) \right|\right|$$

We will calculate an upper bound on the increment $r_k(H,t+\delta t) - r_k(H,t)$. Using the triangle inequality we get,

$$\begin{aligned} r_k(H,t+\delta t) - r_k(H,t) &= \left|\left| H(t+\delta t) - \sum_{p=0}^{k-1} \frac{(t+\delta t)^p}{p!} L^p(H) \right|\right| - \left|\left| H(t) - \sum_{p=0}^{k-1} \frac{t^p}{p!} L^p(H) \right|\right| \\ &\leq \left|\left| H(t+\delta t) - H(t) - \left(\sum_{p=0}^{k-1} \frac{(t+\delta t)^p}{p!} L^p(H) - \sum_{p=0}^{k-1} \frac{t^p}{p!} L^p(H) \right) \right|\right| \end{aligned}$$

Now,

$$\begin{aligned} H(t+\delta t) &= e^{S(t+\delta t)} He^{-S(t+\delta t)} \\ &= H + [S(t+\delta t), H] + \frac{1}{2!}[S(t+\delta t), [S(t+\delta t), H]] + \cdots \\ &= H + (t+\delta t)[S,H] + \frac{1}{2!}(t+\delta t)^2 [S,[S,H]] + \frac{1}{3!}(t+\delta t)^3 [S,[S,[S,H]]] + \cdots \\ &= H + (t+\delta t)[S,H] + \frac{1}{2!}(t^2 + 2t\delta t)[S,[S,H]] + \frac{1}{3!}(t^3 + 3t^2\delta t)[S,[S,[S,H]]] + \cdots \\ &+ O((\delta t)^2) \\ &= H + t[S,H] + \frac{1}{2!}t^2[S,[S,H]] + \frac{1}{3!}t^3[S,[S,[S,H]]] + \cdots \\ &+ \delta t[S,H] + \frac{1}{2!}2t\delta t[S,[S,H]] + \frac{1}{3!}3t^2\delta t[S,[S,[S,H]]] + \cdots + O((\delta t)^2) \\ &= H + [St,H] + \frac{1}{2!}[St,[St,H]] + \frac{1}{3!}[St,[St,[St,H]]] + \cdots \\ &+ \delta t[S,H] + \delta t[St,[S,H]] + \frac{1}{2!}\delta t[St,[St,[S,H]]] + \cdots + O((\delta t)^2) \\ &= H(t) + \delta t e^{St} L(H) e^{-St} + O((\delta t)^2) \end{aligned}$$

Thus,

$$H(t+\delta t) - H(t) = \delta t e^{St} L(H) e^{-St} + O((\delta t)^2)$$

For any $k \geq 1$ one has

$$\begin{aligned}
&\sum_{p=0}^{k-1} \frac{(t+\delta t)^p}{p!} L^p(H) - \sum_{p=0}^{k-1} \frac{t^p}{p!} L^p(H) \\
= &\sum_{p=0}^{k-1} \left(\frac{(t+\delta t)^p}{p!} - \frac{t^p}{p!} \right) L^p(H) \\
= &\sum_{p=0}^{k-1} \left(\frac{(t+\delta t)^p - t^p}{p!} \right) L^p(H) \\
= &\sum_{p=0}^{k-1} \left(\frac{pt^{p-1}\delta t + (p(p-1)/2)t^{p-2}(\delta t)^2 + \cdots}{p!} \right) L^p(H) \\
= &\ \delta t \sum_{p=0}^{k-1} \frac{t^{p-1}}{(p-1)!} L^p(H) + O((\delta t)^2) \\
= &\ \delta t \sum_{p=0}^{k-1} \frac{t^{p-1}}{(p-1)!} L^{p-1}(L(H)) + O((\delta t)^2) \\
= &\ \delta t \sum_{p=0}^{k-2} \frac{t^p}{p!} L^p(L(H)) + O((\delta t)^2)
\end{aligned}$$

Therefore,

$$\begin{aligned}
r_k(H, t+\delta t) - r_k(H,t) &\leq \left\| H(t+\delta t) - H(t) - \left(\sum_{p=0}^{k-1} \frac{(t+\delta t)^p}{p!} L^p(H) - \sum_{p=0}^{k-1} \frac{t^p}{p!} L^p(H) \right) \right\| \\
&= \left\| \delta t e^{St} L(H) e^{-St} - \delta t \sum_{p=0}^{k-2} \frac{t^p}{p!} L^p(L(H)) \right\| + O((\delta t)^2) \\
&= \delta t \left\| e^{St} L(H) e^{-St} - \sum_{p=0}^{k-2} \frac{t^p}{p!} L^p(L(H)) \right\| + O((\delta t)^2) \\
&= \delta t r_{k-1}(L(H), t) + O((\delta t)^2)
\end{aligned}$$

Now take $t = 0, \delta t, 2\delta t, 3\delta t, \cdots$.

$$\begin{aligned}
r_k(H, \delta t) - r_k(H, 0) &\leq \delta t r_{k-1}(L(H), 0) + O((\delta t)^2) \\
r_k(H, 2\delta t) - r_k(H, \delta t) &\leq \delta t r_{k-1}(L(H), \delta t) + O((\delta t)^2) \\
r_k(H, 3\delta t) - r_k(H, 2\delta t) &\leq \delta t r_{k-1}(L(H), 2\delta t) + O((\delta t)^2) \\
&\vdots \\
r_k(H, n\delta t) - r_k(H, (n-1)\delta t) &\leq \delta t r_{k-1}(L(H), (n-1)\delta t) + O((\delta t)^2)
\end{aligned}$$

By adding all those inequalities we get,

$$\begin{aligned} r_k(H,n\delta t)-r_k(H,0) &\leq \delta t\sum_{l=0}^{n-1} r_{k-1}(L(H),l\delta t)+nO((\delta t)^2) \\ r_k(H,n\delta t) &\leq \delta t\sum_{l=0}^{n-1} r_{k-1}(L(H),l\delta t)+n\delta t O(\delta t) \end{aligned}$$

Finally we take the limit $\delta t \to 0$.

$$r_k(H,s) \leq \int_0^s r_{k-1}(L(H),t)dt$$

Using this recursive relation, one can obtain the following.

$$\begin{aligned} r_k(H,s) &\leq \int_0^s r_{k-1}(L(H),t)dt \\ &\leq \int_0^s \left(\int_0^s r_{k-2}(L^2(H),t)dt\right)dt \\ &\leq \int_0^s \left(\int_0^s \left(\int_0^s r_{k-3}(L^3(H),t)dt\right)dt\right)dt \\ &\leq \int_0^s \left(\int_0^s \left(\int_0^s \cdots \int_0^s r_0(L^k(H),t)dt\cdots dt\right)dt\right)dt \\ &\leq \int_0^s \left(\int_0^s \left(\int_0^s \cdots \int_0^s ||L^k(H)||dt\cdots dt\right)dt\right)dt \\ &\leq ||L^k(H)||\frac{s^k}{k!} \end{aligned}$$

We can finish the proof, by putting $s=1$.

$$\begin{aligned} r_k(H,1) &\leq ||L^k(H)||\frac{1}{k!} \\ r_k(H) &\leq \frac{1}{k!}||L^k(H)|| \end{aligned}$$

□

Lemma III.2.2. *([2], p.3) Let S and H be any $O(1)$-local operators acting on n qubits with $S=J_SA$ and $H=J_HB$ where J_S,J_H are constants and $||A||,||B||\leq 1$. Then for any $k=O(1)$ one has $||L^k(H)||=O(J_S^kJ_H)$*

Proof. Since S and H are $O(1)$ local operators, we can write them as $S=\sum_{i=1}^{K'} S_i$ and $H=\sum_{j=1}^{K} H_j$ such that any S_i and H_j act on $O(1)$ qubits and any qubit is acted on by $O(1)$ operators

S_i, H_J. Then $L^k(H) = \left[\sum_{i=1}^{K'} S_i, \left[\sum_{i=1}^{K'} S_i, \cdots \left[\sum_{i=1}^{K'} S_i, \sum_{j=1}^{K''} H_j\right]\right]\right] = \sum_{i_1, i_2, \cdots, i_k, j} [S_{i_1}, [S_{i_2}, \cdots [S_{i_k}, H_j]]]$. Each term $[S_{i_1}, [S_{i_2}, \cdots [S_{i_k}, H_j]]]$ is an operator of $O(J_S^k J_H)$. Therefore, by applying the triangle inequality we get $||L^k(H)|| = O(J_S^k J_H)$. □

APPENDIX B

PROOF OF MAIN THEOREMS

We will give the detailed proof for our main theorems. For simplicity we will skip some of the subscripts and superscripts. For example, we will denote the effective Hamiltonian H_{eff} by H, S_u by S and so on.

Theorem III.3.1. *Let the target Hamiltonian be* $H_{target} = \frac{J}{2}(AB+BA)$ *where* $||A||, ||B|| \leq 1$. *Introduce a two dimensional mediator Hilbert space* $\mathcal{H} = span\{|0\rangle, |1\rangle\}$ *over* $\mathbb{C}$. *If we define the simulator Hamiltonian* $H = H_0 + V$, *with*

$$\begin{aligned} H_0 &= J\varepsilon^{-2} Q_u \\ V &= V_1 + V_{extra} \\ V_1 &= \frac{J\varepsilon^{-1}}{\sqrt{2}} \sigma_x^u \otimes (-A+B) \\ V_{extra} &= (J/2)(A^2+B^2) \end{aligned}$$

then $Pe^S He^{-S} P$ *is close to* $H_{target} = \frac{J}{2}(AB+BA)$ *where* $S = -i\frac{\varepsilon}{\sqrt{2}}\sigma_y^u \otimes (-A+B)$.

Proof. Let $S = -i\frac{\varepsilon}{\sqrt{2}}\sigma_y^u \otimes (-A+B)$. Then we get([13]),

$$e^S He^{-S} = H + [S,H] + \frac{1}{2}[S,[S,H]] + \frac{1}{3!}[S,[S,[S,H]]] + \cdots$$

Now we will compute $[S,H], [S,[S,H]], [S,[S,[S,H]]], \cdots$.

$$\begin{aligned} [S,H_0] &= [S, J\varepsilon^{-2} Q_u] \\ &= \left[-\frac{i\varepsilon}{\sqrt{2}} \sigma_y^u \otimes (-A+B), J\varepsilon^{-2} Q_u \right] \\ &= -\frac{iJ\varepsilon^{-1}}{\sqrt{2}} \left[\sigma_y^u \otimes (-A+B), Q_u \right] \\ &= -\frac{iJ\varepsilon^{-1}}{\sqrt{2}} \left[\sigma_y^u, Q_u \right] \otimes (-A+B) \\ &= -\frac{iJ\varepsilon^{-1}}{\sqrt{2}} (-i) \sigma_x^u \otimes (-A+B) \\ &= -\frac{J\varepsilon^{-1}}{\sqrt{2}} \sigma_x^u \otimes (-A+B) \end{aligned}$$

$$
\begin{aligned}
[S,[S,H_0]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u\otimes(-A+B), -\frac{i\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u\otimes(-A+B)\right] \\
&= \frac{iJ}{2}\left[\sigma_y^u\otimes(-A+B), \sigma_x^u\otimes(-A+B)\right] \\
&= \frac{iJ}{2}\left[\sigma_y^u, \sigma_x^u\right]\otimes(-A+B)^2 \\
&= \frac{iJ}{2}(-2i)\sigma_z^u\otimes(-A+B)^2 \\
&= J\sigma_z^u\otimes(-A+B)^2
\end{aligned}
$$

$$
\begin{aligned}
[S,[S,[S,H_0]]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u\otimes(-A+B), J\sigma_z^u\otimes(-A+B)^2\right] \\
&= -\frac{iJ\varepsilon}{\sqrt{2}}\left[\sigma_y^u, \sigma_z^u\right]\otimes(-A+B)^3 \\
&= -\frac{iJ\varepsilon}{\sqrt{2}}\cdot 2i\sigma_x^u\otimes(-A+B)^3 \\
&= \sqrt{2}J\varepsilon\sigma_x^u\otimes(-A+B)^3
\end{aligned}
$$

$$
\begin{aligned}
[S,V_1] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u\otimes(-A+B), \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u\otimes(-A+B)\right] = -J\sigma_z^u\otimes(-A+B)^2 \\
[S,[S,V_1]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u\otimes(-A+B), -J\sigma_z^u\otimes(-A+B)^2\right] = -\sqrt{2}J\varepsilon\sigma_x^u\otimes(-A+B)^3 \\
[S,[S,[S,V_1]]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u\otimes(-A+B), -J\varepsilon\sigma_x^u\otimes(-A+B)^3\right] = \sqrt{2}J\varepsilon^2\sigma_z^u\otimes(-A+B)^4
\end{aligned}
$$

The calculations for $[S,V_1]$, $[S,[S,V_1]]$ and $[S,[S,[S,V_1]]]$ are similar to the calculations for $[S,[S,H_0]]$, and $[S,[S,[S,H_0]]]$.

$$
\begin{aligned}
[S,V_{\text{extra}}] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u\otimes(-A+B), (J/2)(A^2+B^2)\right] \\
&= -\frac{iJ\varepsilon}{2\sqrt{2}}\left[\sigma_y^u\otimes(-A+B), A^2+B^2\right] \\
&= O(J\varepsilon)
\end{aligned}
$$

So, $[S,[S,V_{\text{extra}}] = O(J\varepsilon^2)$ and $[S,[S,[S,V_{\text{extra}}]]] = O(J\varepsilon^3)$ Hence,

$$
\begin{aligned}
H &= J\varepsilon^{-2}Q_u + \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u \otimes (-A+B) + (J/2)(A^2+B^2) \\
[S,H] &= [S,H_0] + [S,V_1] + [S,V_{\text{extra}}] \\
&= -\frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u \otimes (-A+B) - J\sigma_z^u \otimes (-A+B)^2 + O(J\varepsilon) \\
[S,[S,H]] &= [S,[S,H_0]] + [S,[S,V_1]] + [S,[S,V_{\text{extra}}]] \\
&= J\sigma_z^u \otimes (-A+B)^2 - \sqrt{2}J\varepsilon\sigma_x^u \otimes (-A+B)^3 + O(J\varepsilon^2) \\
[S,[S,[S,H]]] &= [S,[S,[S,H_0]]] + [S,[S,[S,V_1]]] + [S,[S,[S,V_{\text{extra}}]]] \\
&= \sqrt{2}J\varepsilon\sigma_x^u \otimes (-A+B)^3 + \sqrt{2}J\varepsilon^2\sigma_z^u \otimes (-A+B)^4 + O(J\varepsilon^3)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
e^S He^{-S} &= H + [S,H] + \frac{1}{2}[S,[S,H]] + \frac{1}{3!}[S,[S,[S,H]]] + \cdots \\
&= J\varepsilon^{-2}Q_u + (J/2)(A^2+B^2) - \frac{J}{2}\sigma_z^u \otimes (-A+B)^2 - \frac{\sqrt{2}J\varepsilon}{3}\sigma_x^u \otimes (-A+B)^3 + \cdots \\
&= J\varepsilon^{-2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + (J/2)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes (A^2+B^2) - \frac{J}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes (-A+B)^2 - O(J\varepsilon) + \cdots \\
&= \begin{pmatrix} \frac{J}{2}(AB+BA) & 0 \\ 0 & J\varepsilon^{-2}I + J(A^2+B^2-(AB+BA)/2) \end{pmatrix} - O(J\varepsilon) + \cdots \\
&= \begin{pmatrix} \frac{J}{2}(AB+BA) & 0 \\ 0 & J\varepsilon^{-2}I + O(J) \end{pmatrix} - O(J\varepsilon) + \cdots
\end{aligned}
$$

Therefore, $Pe^S He^{-S}P$ is close to $H_{\text{target}} = \frac{J}{2}(AB+BA)$.

□

Theorem III.3.2. *Let the target Hamiltonian be $H_{target} = JABC$ where A, B and C act on non overlapping Hilbert spaces and $||A||, ||B||, ||C|| \leq 1$. Introduce a 2-dimensional mediator Hilbert space span$\{|0\rangle, |1\rangle\}$ over $\mathbb{C}$. If we define the simulator Hamiltonian $H = H_0 + V$, with*

$$
\begin{aligned}
H_0 &= J\varepsilon^{-3}Q_u \\
V_d &= -J\varepsilon^{-2}Q_u \otimes C \\
V_{od} &= J\frac{\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u \otimes (-A+B) \\
V_{extra} &= J\varepsilon^{-1}(-A+B)^2/2 + J(A^2+B^2)C/2
\end{aligned}
$$

and $S = -\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R$ where $R = (-A+B)\{I + \varepsilon C + \varepsilon^2 C^2 - \frac{2\varepsilon^2}{3}(-A+B)^2\}$ then $Pe^S He^{-S}P$ is ε close to $H_{target} = JABC$.

Proof. We know([13]),

$$e^S H e^{-S} = H + [S,H] + \frac{1}{2}[S,[S,H]] + \frac{1}{3!}[S,[S,[S,H]]] + \cdots$$

Now we will compute $[S,H],[S,[S,H]],[S,[S,[S,H]]],\cdots$ using the fact that A and B commute since they are acting on non overlapping subspaces.

$$\begin{aligned}
H_0 &= J\varepsilon^{-3}Q_u \\
[S,H_0] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R, J\varepsilon^{-3}Q_u\right] \\
&= -\frac{iJ\varepsilon^{-2}}{\sqrt{2}}\left[\sigma_y^u \otimes R, Q_u\right] \\
&= -\frac{iJ\varepsilon^{-2}}{\sqrt{2}}\left[\sigma_y^u, Q_u\right] \otimes R \\
&= -\frac{iJ\varepsilon^{-2}}{\sqrt{2}}(-i)\sigma_x^u \otimes R \\
&= -\frac{J\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u \otimes R
\end{aligned}$$

$$\begin{aligned}
[S,[S,H_0]] &= \frac{iJ\varepsilon^{-1}}{2}\left[\sigma_y^u \otimes R, \sigma_x^u \otimes R\right] \\
&= \frac{iJ\varepsilon^{-1}}{2}\left[\sigma_y^u, \sigma_x^u\right] \otimes R^2 \\
&= \frac{iJ\varepsilon^{-1}}{2}(-2i)\sigma_z^u \otimes R^2 \\
&= J\varepsilon^{-1}\sigma_z^u \otimes R^2
\end{aligned}$$

$$\begin{aligned}
[S,[S,[S,H_0]]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R, J\varepsilon^{-1}\sigma_z^u \otimes R^2\right] \\
&= -\frac{iJ}{\sqrt{2}}\left[\sigma_y^u, \sigma_z^u\right] \otimes R^3 \\
&= -\frac{iJ}{\sqrt{2}} \cdot 2i\sigma_x^u \otimes R^3 \\
&= \sqrt{2}J\sigma_x^u \otimes R^3
\end{aligned}$$

$$
\begin{aligned}
V_{\mathrm{d}} &= -J\varepsilon^{-2}Q_u \otimes C \\
[S,V_d] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R, -J\varepsilon^{-2}Q_u \otimes C\right] \\
&= \frac{iJ\varepsilon^{-1}}{\sqrt{2}}\left[\sigma_y^u \otimes R, Q_u \otimes C\right] \\
&= \frac{iJ\varepsilon^{-1}}{\sqrt{2}}\left[\sigma_y^u, Q_u\right] \otimes RC \\
&= \frac{iJ\varepsilon^{-1}}{\sqrt{2}}(-i)\sigma_x^u \otimes RC \\
&= \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u \otimes RC
\end{aligned}
$$

$$
\begin{aligned}
[S,[S,V_d]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R, \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u \otimes RC\right] \\
&= -\frac{iJ}{2}\left[\sigma_y^u \otimes R, \sigma_x^u \otimes RC\right] \\
&= -\frac{iJ}{2}\left[\sigma_y^u, \sigma_x^u\right] \otimes R^2C \\
&= -\frac{iJ}{2}(-2i)\sigma_z^u \otimes R^2C \\
&= -J\sigma_z^u \otimes R^2C
\end{aligned}
$$

$$
\begin{aligned}
[S,[S,[S,V_d]]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R, -J\sigma_z^u \otimes R^2C\right] \\
&= \frac{iJ\varepsilon}{\sqrt{2}}\left[\sigma_y^u \otimes R, \sigma_z^u \otimes R^2C\right] \\
&= \frac{iJ\varepsilon}{\sqrt{2}}\left[\sigma_y^u, \sigma_z^u\right] \otimes R^3C \\
&= \frac{iJ\varepsilon}{\sqrt{2}}2i\sigma_x^u \otimes R^3C \\
&= -\sqrt{2}J\varepsilon\sigma_x^u \otimes R^3C
\end{aligned}
$$

$$
\begin{aligned}
V_{\text{od}} &= \frac{J\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u \otimes (-A+B) \\
[S, V_{\text{od}}] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R, \frac{J\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u \otimes (-A+B)\right] \\
&= -\frac{iJ\varepsilon^{-1}}{2}\left[\sigma_y^u \otimes R, \sigma_x^u \otimes (-A+B)\right] \\
&= -\frac{iJ\varepsilon^{-1}}{2}\left[\sigma_y^u, \sigma_x^u\right] \otimes R(-A+B) \\
&= -\frac{iJ\varepsilon^{-1}}{2}(-2i)\sigma_z^u \otimes R(-A+B) \\
&= -J\varepsilon^{-1}\sigma_z^u \otimes R(-A+B)
\end{aligned}
$$

$$
\begin{aligned}
[S,[S,V_{\text{od}}]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R, -J\varepsilon^{-1}\sigma_z^u \otimes R(-A+B)\right] \\
&= \frac{iJ}{\sqrt{2}}\left[\sigma_y^u \otimes R, \sigma_z^u \otimes R(-A+B)\right] \\
&= \frac{iJ}{\sqrt{2}}\left[\sigma_y^u, \sigma_z^u\right] \otimes R^2(-A+B) \\
&= \frac{iJ}{\sqrt{2}}2i\sigma_x^u \otimes R^2(-A+B) \\
&= -\sqrt{2}J\sigma_x^u \otimes R^2(-A+B)
\end{aligned}
$$

$$
\begin{aligned}
[S,[S,[S,V_{\text{od}}]]] &= \left[-\frac{i\varepsilon}{\sqrt{2}}\sigma_y^u \otimes R, -\sqrt{2}J\sigma_x^u \otimes R^2(-A+B)\right] \\
&= iJ\varepsilon\left[\sigma_y^u \otimes R, \sigma_x^u \otimes R^2(-A+B)\right] \\
&= iJ\varepsilon\left[\sigma_y^u, \sigma_x^u\right] \otimes R^3(-A+B) \\
&= iJ\varepsilon(-2i)\sigma_z^u \otimes R^3(-A+B) \\
&= 2J\varepsilon\sigma_z^u \otimes R^3(-A+B)
\end{aligned}
$$

Since A, B, C commute, we get

$$
[S, V_{\text{extra}}] = [S,[S,V_{\text{extra}}] = [S,[S,[S,V_{\text{extra}}]]] = 0
$$

Suppose $H + [S,H] + \frac{1}{2}[S,[S,H]] + \frac{1}{3!}[S,[S,[S,H]]] = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} + O(J\varepsilon)$. Then using $H =$

$H_0+V_\mathrm{d}+V_\mathrm{od}+V_\mathrm{extra}$ and form the above calculations we get,

$$\begin{aligned}
M_{11} &= \frac{1}{2}J\varepsilon^{-1}R^2-\frac{1}{2}JR^2C-J\varepsilon^{-1}R(-A+B)+\frac{1}{2}J\varepsilon^{-1}(-A+B)^2+\frac{1}{2}J(A^2+B^2)C+O(J\varepsilon)\\
&= \frac{J}{2}\varepsilon^{-1}\left(R^2-2R(-A+B)+(-A+B)^2\right)+\frac{J}{2}\left((A^2+B^2)C-R^2C\right)+O(J\varepsilon)\\
&= \frac{J}{2}\varepsilon^{-1}(R+A-B)^2+\frac{J}{2}\left((A^2+B^2)-R^2\right)C+O(J\varepsilon)\\
&= \frac{J}{2}\varepsilon^{-1}\left(\varepsilon C+\varepsilon^2C^2-\frac{2\varepsilon^2}{3}(-A+B)^2\right)^2+\frac{J}{2}\left((A^2+B^2)-(-A+B)^2+O(\varepsilon)\right)C+O(J\varepsilon)\\
&= \frac{J}{2}\varepsilon\left(C+\varepsilon-\frac{2\varepsilon}{3}(-A+B)^2\right)^2+\frac{J}{2}(2AB+O(\varepsilon))C+O(J\varepsilon)\\
&= JABC+O(J\varepsilon)
\end{aligned}$$

$$M_{12}=\frac{J\varepsilon^{-2}}{\sqrt{2}}(-A+B)-\frac{J\varepsilon^{-2}}{\sqrt{2}}R+\frac{1}{6}\sqrt{2}JR^3+\frac{J\varepsilon^{-1}}{\sqrt{2}}RC-\frac{1}{2}\sqrt{2}JR^2(-A+B)+O(J\varepsilon)\quad \text{(IV.1)}$$

But,

$$\begin{aligned}
-\frac{J\varepsilon^{-2}}{\sqrt{2}}R &= -\frac{J\varepsilon^{-2}}{\sqrt{2}}\left((-A+B)\{I+\varepsilon C+\varepsilon^2C^2-\frac{2\varepsilon^2}{3}(-A+B)^2\}\right)\\
&= -\frac{J\varepsilon^{-2}}{\sqrt{2}}(-A+B)-\frac{J\varepsilon^{-1}}{\sqrt{2}}(-A+B)C-\frac{J}{\sqrt{2}}(-A+B)C^2+\frac{2J}{3\sqrt{2}}(-A+B)^3\\
\frac{1}{6}\sqrt{2}JR^3 &= \frac{J}{3\sqrt{2}}(-A+B)^3+O(J\varepsilon)\\
\frac{J\varepsilon^{-1}}{\sqrt{2}}RC &= \frac{J\varepsilon^{-1}}{\sqrt{2}}(-A+B)C+\frac{J}{\sqrt{2}}(-A+B)C^2+O(J\varepsilon)\\
-\frac{1}{2}\sqrt{2}JR^2(-A+B) &= -\frac{J}{\sqrt{2}}(-A+B)^3+O(J\varepsilon)
\end{aligned}$$

By putting these expressions in equation (IV.1) we get, $M_{12}=O(J\varepsilon)$. We can easily verify that $M_{21}=M_{12}$. Therefore, $M_{21}=M_{12}=O(J\varepsilon)$. And

$$\begin{aligned}
M_{22} &= J\varepsilon^{-3}+\frac{J\varepsilon^{-1}}{2}(-A+B)^2+\frac{J}{2}(A^2+B^2)C+\frac{J\varepsilon^{-1}}{2}R^2\\
&- J\varepsilon^{-2}C-\frac{J}{2}R^2C-J\varepsilon^{-1}R(-A+B)+O(J\varepsilon)\\
&= J\varepsilon^{-3}+O(J\varepsilon^{-2})
\end{aligned}$$

Hence,

$$H+[S,H]+\frac{1}{2}[S,[S,H]]+\frac{1}{3!}[S,[S,[S,H]]]+\cdots=\begin{pmatrix} JABC & 0\\ 0 & J\varepsilon^{-3}I+O(J\varepsilon^{-2})\end{pmatrix}+O(J\varepsilon)$$

Therefore, $Pe^{S}He^{-S}P$ is ε close to $H_{\text{target}} = JABC$.

□

Theorem III.3.3. *Let $H_{target} = \sum_u H^u_{target} + H_{else}$ where H^u_{target}s are of form $\frac{J}{2}(AB+BA)$ or $JABC$. If $H = \sum_u H^u + H_{else}$, where H^u is the simulator Hamiltonian for H^u_{target}, constructed using Theorem (III.3.1) and Theorem (III.3.2), then the ground state energy of H approximates the ground state energy of H_{target}.*

Proof. First, we will show that $\lambda(H) \geq \lambda(H_{\text{target}}) + O(J\varepsilon)$. For subdivision gadget,

$$
\begin{aligned}
e^{S^u}H^u e^{-S^u} - I^u \otimes H^u_{\text{target}} &= \begin{pmatrix} \frac{J}{2}(AB+BA) & 0 \\ 0 & J\varepsilon^{-2}I + O(J) \end{pmatrix} + O(J\varepsilon) - \begin{pmatrix} \frac{J}{2}(AB+BA) & 0 \\ 0 & \frac{J}{2}(AB+BA) \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 \\ 0 & J\varepsilon^{-2}I + O(J) - \frac{J}{2}(AB+BA) \end{pmatrix} + O(J\varepsilon)
\end{aligned}
$$

and for 3-to-2 gadget,

$$
\begin{aligned}
e^{S^u}H^u e^{-S^u} - I^u \otimes H^u_{\text{target}} &= \begin{pmatrix} JABC & 0 \\ 0 & J\varepsilon^{-3}I + O(J\varepsilon^{-2}) \end{pmatrix} + O(J\varepsilon) - \begin{pmatrix} JABC & 0 \\ 0 & JABC \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 \\ 0 & J\varepsilon^{-3}I + O(J\varepsilon^{-2}) - JABC \end{pmatrix} + O(J\varepsilon)
\end{aligned}
$$

Since $\varepsilon << 1$, we have $J\varepsilon^{-2}I + O(J) - \frac{J}{2}(AB+BA) \geq 0$ and $J\varepsilon^{-3}I + O(J\varepsilon^{-2}) - JABC \geq 0$ which imply that $e^{S^u}H^u e^{-S^u} - I^u \otimes H^u_{\text{target}} \geq O(J\varepsilon)$. Hence,

$$
e^{S^u}H^u e^{-S^u} \geq I^u \otimes H^u_{\text{target}} + O(J\varepsilon)
$$

implies,

$$
H^u \geq e^{-S^u}\left(I^u \otimes H^u_{\text{target}}\right)e^{S^u} + O(J\varepsilon) \qquad \text{(IV.2)}
$$

For subdivision gadget,

$$
\begin{aligned}
\left|\left|\left[S^u, I^u \otimes H^u_{\text{target}}\right]\right|\right| &= \left|\left|\left[-i\varepsilon\sigma^u_y \otimes (-A+B), \frac{J}{2}(AB+BA)\right]\right|\right| \\
&= J\varepsilon\left|\left|\left[-i\sigma^u_y \otimes (-A+B), \frac{J}{2}(AB+BA)\right]\right|\right| \\
&= O(J\varepsilon)
\end{aligned}
$$

For 3-to-2 gadget,

$$\begin{aligned} |||[S^u, I^u \otimes H^u_{\text{target}}]||| &= \left|\left|\left|\left[-\frac{i\varepsilon}{\sqrt{2}}\sigma^u_y \otimes R, JABC\right]\right|\right|\right| \\ &= -\frac{J\varepsilon}{\sqrt{2}}|||[i\sigma^u_y \otimes R, I^u \otimes JABC]||| \\ &= O(J\varepsilon) \end{aligned}$$

Hence, Lemma (III.2.1) implies,

$$\left|\left|e^{-S^u}\left(I^u \otimes H^u_{\text{target}}\right)e^{S^u} - I^u \otimes H^u_{\text{target}}\right|\right| \leq |||[S^u, I^u \otimes H^u_{\text{target}}]||| = O(J\varepsilon)$$

So we can write

$$e^{-S^u}\left(I^u \otimes H^u_{\text{target}}\right)e^{S^u} = I^u \otimes H^u_{\text{target}} + \left[S^u, I^u \otimes H^u_{\text{target}}\right] + \left[S^u\left[S^u, I^u \otimes H^u_{\text{target}}\right]\right] + \cdots = I^u \otimes H^u_{\text{target}} + O(J\varepsilon)$$

Therefore, from inequality (IV.2), we get

$$\begin{aligned} H^u &\geq I^u \otimes H^u_{\text{target}} + O(J\varepsilon) \\ \sum H^u &\geq \sum I^u \otimes H^u_{\text{target}} + O(J\varepsilon) \\ H &\geq I \otimes H_{\text{target}} + O(nJ\varepsilon) \\ \lambda(H) &\geq \lambda(I \otimes H_{\text{target}}) + O(nJ\varepsilon) \\ \lambda(H) &\geq \lambda(H_{\text{target}}) + O(nJ\varepsilon) \end{aligned}$$

Now we will show that $\lambda(H) \leq \lambda(H_{\text{target}}) + O(J\varepsilon)$ using $||Pe^S He^{-S}P - H_{\text{target}}|| = O(nJ\varepsilon)$ where $P = \otimes_u P^u$ and $S = \sum_u S^u$. We get,

$$\begin{aligned} \lambda(H) &= \lambda(e^S He^{-S}) \\ &\leq \lambda(Pe^S He^{-S}P) \\ &= \lambda(H_{\text{target}}) + O(nJ\varepsilon) \end{aligned}$$

We will complete the proof by showing that $||Pe^S He^{-S}P - H_{\text{target}}|| = O(nJ\varepsilon)$.

We have,

$$
\begin{aligned}
e^S H e^{-S} &= e^{\sum_u S^u}(H^1+H^2+\cdots+H^n)e^{-\sum_u S^u} \\
&= \left(H^1+\left[\sum_u S^u, H^1\right]+\left[\sum_u S^u,\left[\sum_u S^u, H^1\right]\right]+\cdots\right) \\
&+ \left(H^2+\left[\sum_u S^u, H^2\right]+\left[\sum_u S^u,\left[\sum_u S^u, H^2\right]\right]+\cdots\right) \\
&+ \cdots \\
&= (H^1+[S^1,H^1]+[S^1,[S^1,H^1]]+\cdots)+(H^2+[S^2,H^2]+[S^2,[S^2,H^2]]+\cdots) \\
&+ (H^3+[S^3,H^3]+[S^3,[S^3,H^3]]+\cdots)+\cdots \\
&+ \sum_{u\neq v}[S^u,H^v]+\sum_{\text{not } u=v=w}[S^u,[S^v,H^w]]+O(J\varepsilon)
\end{aligned}
$$

We will show that the cross-gadget terms does not contribute anything when ε goes to zero. Recall, the simulator Hamiltonian for a subdivision gadget is $H=H_0+V$, with

$$
\begin{aligned}
H_0 &= J\varepsilon^{-2}Q_u \\
V &= V_1+V_{\text{extra}} \\
V_1 &= \frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u\otimes(-A+B) \\
V_{\text{extra}} &= (J/2)(A^2+B^2)
\end{aligned}
$$

and the simulator Hamiltonian for a 3-to-2 gadget is $H=H_0+V$, with

$$
\begin{aligned}
H_0 &= \varepsilon^{-3}Q_u\otimes I \\
V_{\text{d}} &= -\varepsilon^{-2}Q_u\otimes C \\
V_{\text{od}} &= \frac{\varepsilon^{-2}}{\sqrt{2}}\sigma_x^u\otimes(-A+B) \\
V_{\text{extra}} &= \varepsilon^{-1}(-A+B)^2/2+(A^2+B^2)C/2
\end{aligned}
$$

We will discuss the commutator of S and each of these terms separately. Suppose $u\neq v$. Since

$[S^\nu, Q_u] = 0$, we get, $[S^\nu, H_0^u] = 0$. Next we will show that $P[S^\nu, V_1^u]P = 0$.

$$\begin{aligned}
S^\nu V_1^u &= \left(-i\frac{\varepsilon}{\sqrt{2}}Y_\nu \otimes (-A^\nu + B^\nu)\right)\left(\frac{J\varepsilon^{-1}}{\sqrt{2}}\sigma_x^u \otimes (-A^u + B^u)\right) \\
&= \frac{-iJ}{2}(Y_\nu \otimes (-A^\nu + B^\nu))(\sigma_x^u \otimes (-A^u + B^u)) \\
&= \frac{-iJ}{2}(Y_\nu \otimes I_u \otimes (-A^\nu + B^\nu))(I_\nu \otimes \sigma_x^u \otimes (-A^u + B^u)) \\
&= \frac{-iJ}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \sigma_x^u \otimes (-A^\nu + B^\nu)(-A^u + B^u) \\
&= \frac{-J}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \sigma_x^u \otimes (-A^\nu + B^\nu)(-A^u + B^u) \\
&= \frac{-J}{2}\begin{pmatrix} 0 & \sigma_x^u \otimes (-A^\nu + B^\nu)(-A^u + B^u) \\ -\sigma_x^u \otimes (-A^\nu + B^\nu)(-A^u + B^u) & 0 \end{pmatrix}
\end{aligned}$$

Hence, $PS^\nu V_1^u P = 0$. Similar calculations yield $PV_1^u S^\nu P = 0$. Therefore, $P[S^\nu, V_1^u]P = 0$. From this calculations we observe that each time we apply S_ν, it flips the mediator bit. So if we apply S_ν and P on H then we can write $P[S^\nu, H^u]P = 0$. Now we will compute $[S^\nu, [S^\nu, H^u]]$. Since $[S^\nu, H_0^u] = 0$, clearly $[S^\nu, [S^\nu, H_0^u]] = 0$. For subdivision gadget, $[S^\nu, [S^\nu, V_1^u]] = O(J\varepsilon)$ and $[S^\nu, [S^\nu, V_{\text{extra}}^u]] = O(J\varepsilon^2)$. For 3-to-2 gadget, we also have $[S^\nu, [S^\nu, V_{\text{extra}}^u]] = O(J\varepsilon)$. We will explicitly calculate $[S^\nu, [S^\nu, V_{\text{d}}^u]]$ and $[S^\nu, [S^\nu, V_{\text{od}}^u]]$

$$\begin{aligned}
S^\nu S^\nu V_{\text{d}}^u &= \left(-i\frac{\varepsilon}{\sqrt{2}}Y_\nu \otimes (-A^\nu + B^\nu)\right)\left(-i\frac{\varepsilon}{\sqrt{2}}Y_\nu \otimes (-A^\nu + B^\nu)\right)(-J\varepsilon^{-2}Q_u \otimes C^u) \\
&= \frac{-J}{2}(Y_\nu \otimes (-A^\nu + B^\nu))(Y_\nu \otimes (-A^\nu + B^\nu))(Q_u \otimes C^u) \\
&= \frac{-J}{2}(I_u \otimes Y_\nu \otimes (-A^\nu + B^\nu))(I_u \otimes Y_\nu \otimes (-A^\nu + B^\nu))(Q_u \otimes C^u \otimes I_\nu) \\
&= \frac{-J}{2}(Q_u \otimes C^u \otimes I_\nu \otimes (-A^\nu + B^\nu)^2) \\
&= \frac{-J}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes Q_u \otimes C^u \otimes I_\nu \otimes (-A^\nu + B^\nu)^2 \\
&= \frac{-J}{2}\begin{pmatrix} 0 & 0 \\ 0 & Q_u \otimes C^u \otimes I_\nu \otimes (-A^\nu + B^\nu)^2 \end{pmatrix}
\end{aligned}$$

Hence $PS^\nu S^\nu V_{\text{d}}^u P = 0$. Similarly we can calculate all the terms in $[S^\nu, [S^\nu, V_{\text{d}}^u]]$ and $[S^\nu, [S^\nu, V_{\text{od}}^u]]$, From all these calculations we can conclude that $P[S^\nu, [S^\nu, V_{\text{d}}^u]]P = 0$ and $P[S^\nu, [S^\nu, V_{\text{od}}^u]]P = 0$

Therefore,

$$
\begin{aligned}
Pe^{S}He^{-S}P &= \otimes_u P^u \left[e^{\sum_u S^u} (H^1 + H^2 + \cdots + H^n) e^{-\sum_u S^u} \right] \otimes_u P^u \\
&= \otimes_u P^u \left(H^1 + \left[S^1, H^1\right] + \left[S^1, \left[S^1, H^1\right]\right] + \cdots \right) \otimes_u P^u \\
&+ \otimes_u P^u \left(H^2 + \left[S^2, H^2\right] + \left[S^2, \left[S^2, H^2\right]\right] + \cdots \right) \otimes_u P^u \\
&+ \cdots \\
&+ \otimes_u P^u \left(\sum_{u \neq v} [S^u, H^v] \right) \otimes_u P^u + \otimes_u P^u \left(\sum_{\text{not} u = v = w} [S^u, [S^v, H^w]] \right) \otimes_u P^u \\
&+ \cdots \\
&= H^1_{\text{target}} + H^2_{\text{target}} + \cdots + H^n_{\text{target}} + O(nJ\varepsilon) \\
&= H_{\text{target}} + O(nJ\varepsilon) \\
||Pe^{S}He^{-S}P - H_{\text{target}}|| &= O(nJ\varepsilon)
\end{aligned}
$$

□

APPENDIX C

MAPLE CODE FOR NUMERICAL VERIFICATION

Program code for numerical verification of 3-to-2 gadget.

```
> with(linalg);
> kronprod:=proc(A,B) (This procedure is taken from internet)
local Ap, Bp, i,j;
if nargs > 2 then RETURN(kronprod(kronprod(A,B),args[3..nargs])) fi;
if type(A,{vector,list(algebraic)}) and
type(B,{vector,list(algebraic)}) then
# vector x vector = vector
vector([seq(seq(A[i]*B[j], j=1..linalg[vectdim](B)),
i=1..linalg[vectdim](A))])
else # otherwise result is matrix
if type(A,matrix) then Ap:= A
elif type(A,listlist) then Ap:= convert(A,matrix)
elif type(A,list) then Ap:= matrix(map(t->[t],A))
elif type(A,specfunc(list,transpose)) then Ap:= matrix([op(A)])
else Ap:= convert(A,matrix)
fi;
if type(B,matrix) then Bp:= B
elif type(B,listlist) then Bp:= convert(B,matrix)
elif type(B,list) then Bp:= matrix(map(t->[t],B))
elif type(B,specfunc(list,transpose)) then Bp:= matrix([op(B)])
else Bp:= convert(B,matrix)
fi;
linalg[stackmatrix](seq(linalg[augment](
seq(linalg[scalarmul](Bp,Ap[i,j]), j = 1 .. linalg[coldim](Ap))),
i = 1 .. linalg[rowdim](Ap)));
fi
end;
> A := matrix([[1.0*(1/5), 2.0*(1/5)], [2.0*(1/5), 3.0*(1/5)]]);
> B := matrix([[2.0*(1/6), 5.0*(1/6)], [1.0*(1/6), 4.0*(1/6)]]);
> C := matrix([[7.0*(1/20), 8.0*(1/20)], [9.0*(1/20), 4.0*(1/20)]]);
> eigenvalues(A);
> eigenvalues(B);
> eigenvalues(C);
> sort([eigenvalues(kronprod(kronprod(A, B), C))]);
> Q := matrix([[0, 0], [0, 1.0]]);
> Id := matrix([[1.0, 0], [0, 1.0]]);
> H[0] := kronprod(kronprod(kronprod(Q, Id), Id), Id);
> V[d] := evalm(-kronprod(kronprod(kronprod(Q, Id), Id), C));
> X := matrix([[0, 1.0], [1.0, 0]]);
> V['od'] := evalm(1.0*(kronprod(kronprod(kronprod(X, evalm(-A)), Id),
Id)+kronprod(kronprod(kronprod(X, Id), evalm(B)), Id))/sqrt(2.0));
```

```
> V[extra1] := evalm(1.0*kronprod(kronprod(Id, evalm((kronprod(evalm(-A),
Id)+kronprod(Id, B))^2)), Id)/(2.0));
> V[extra2] := evalm(1.0*(kronprod(kronprod(kronprod(Id, evalm(A^2)), Id),
C)+kronprod(kronprod(kronprod(Id, Id), evalm(B^2)), C))/(2.0));
> x := 1;
> sort([eigenvalues(x^3*H[0]+x^2*V[d]+x^2*V['od']+x*V[extra1]+V[extra2])]);
> x := 10;
> sort([eigenvalues(x^3*H[0]+x^2*V[d]+x^2*V['od']+x*V[extra1]+V[extra2])]);
> x := 100;
> sort([eigenvalues(x^3*H[0]+x^2*V[d]+x^2*V['od']+x*V[extra1]+V[extra2])]);
> x := 1000;
> sort([eigenvalues(x^3*H[0]+x^2*V[d]+x^2*V['od']+x*V[extra1]+V[extra2])]);
> x := 10000;
> sort([eigenvalues(x^3*H[0]+x^2*V[d]+x^2*V['od']+x*V[extra1]+V[extra2])]);
```

Program code for numerical verification of subdivision gadget.

```
> with(linalg);
> kronprod:=proc(A,B) (This procedure is taken from internet)
> local Ap, Bp, i,j;
> if nargs > 2 then RETURN(kronprod(kronprod(A,B),args[3..nargs])) fi;
> if type(A,{vector,list(algebraic)}) and
> type(B,{vector,list(algebraic)}) then
> # vector x vector = vector
> vector([seq(seq(A[i]*B[j], j=1..linalg[vectdim](B)),
> i=1..linalg[vectdim](A))])
> else # otherwise result is matrix
> if type(A,matrix) then Ap:= A
> elif type(A,listlist) then Ap:= convert(A,matrix)
> elif type(A,list) then Ap:= matrix(map(t->[t],A))
> elif type(A,specfunc(list,transpose)) then Ap:= matrix([op(A)])
> else Ap:= convert(A,matrix)
> fi;
> if type(B,matrix) then Bp:= B
> elif type(B,listlist) then Bp:= convert(B,matrix)
> elif type(B,list) then Bp:= matrix(map(t->[t],B))
> elif type(B,specfunc(list,transpose)) then Bp:= matrix([op(B)])
> else Bp:= convert(B,matrix)
> fi;
> linalg[stackmatrix](seq(linalg[augment](
> seq(linalg[scalarmul](Bp,Ap[i,j]), j = 1 ..  linalg[coldim](Ap))),
> i = 1 ..  linalg[rowdim](Ap)));
> fi
> end;
> A := matrix([[.1, .5], [.4, .1]]);
```

```
> B := matrix([[.2, .5], [.1, .4]]);
> sort([eigenvalues(A)]);
> sort([eigenvalues(B)]);
> sort([eigenvalues(.5*(`&*`(A, B)+`&*`(B, A)))]);
> Q := matrix([[0, 0], [0, 1.0]])
> Id := matrix([[1.0, 0], [0, 1.0]])
> H[0] := kronprod(Q, Id)
> X := matrix([[0, 1.0], [1.0, 0]])
> V[1] := evalm(kronprod(X, evalm(-A/sqrt(2.0)))+kronprod(X, evalm(B/sqrt(2.0)))
> V[2] := evalm(kronprod(Id, evalm((1/2)*A^2))+kronprod(Id, evalm((1/2)*B^2)))
> x := 1
> sort([eigenvalues(x^2*H[0]+x*V[1]+V[2])])
> x := 10
> sort([eigenvalues(x^2*H[0]+x*V[1]+V[2])])
> x := 100
> sort([eigenvalues(x^2*H[0]+x*V[1]+V[2])])
> x := 1000
> sort([eigenvalues(x^2*H[0]+x*V[1]+V[2])])
> x := 10000
> sort([eigenvalues(x^2*H[0]+x*V[1]+V[2])])
```

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