
The Dynamics of the Spectrum by Quantum Walk Algorithm.

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Chapter 1

abstract

Chapter 2

introduction

Quantum computing is one of the most promising emerging scientific and technological fields of the past decades. The theoretical computational advantages of quantum computing allow for valuable applications in fields such as cryptography, chemistry and machine learning. However, quantum computing is no straightforward task: the fundamental issue is to perform high-fidelity operations on a coherent, scalable set of qubits [7]. Another fundamental objective is to manipulate the quantummechanical properties of your qubits as efficiently as possible, using algorithms. Peter Shor’s prime factorization algorithm first showed the potential of quantum algorithms, and present research aims to find the most efficient algorithm for the ground state energy problem in chemistry [11].

This problem is highly relevant, as three percent of the world’s energy output is spent on making fertilizer [9]. We currently rely on a highly outdated, energy-intensive process requiring very large amounts of natural gas. However, there exists an anaerobic bacteria performing a process serving the exact same function while requiring much less energy, utilizing nitrogen fixation with molecules such as FeMoCo. Traditional chemical analyses have not been able to give us an understanding on the details of this process, and as this molecule is highly complex, simulations using classical supercomputers are out of reach. Reiher et al. [9] have shown that quantum computers are, even when taking in account the substantial decoherence and error of current gate computations, able to elucidate chemical processes such as nitrogen fixation in nitrogenase [9]. Current research within quantum computing has not yet been able to provide significant insight into nitrogenase, and this study aims to build towards understanding more complex chemical reactions with quantum computers by examining the efficiency of a quantum walk ground-energy algorithm on the water molecule. If the scientific community succeeds in elucidating nitrogenase, new and more efficient processes of creating fertilizer may be developed, significantly reducing the global carbon footprint.

The most fundamental property of a static molecule is the energy of the molecule in its ground state. Before any other significant conclusions can be drawn about a molecule, the ground state energy must be known and accurately measured. If the field of quantum computing wishes to contribute to the understanding of chemical processes, it must succeed in efficiently retrieving the eigenvalues and eigenstates of the Hamiltonian operator of the molecule. The water molecule is simple enough for a classical computer to simulate and the ground state energy can be determined with the Hartree-Fock method, allowing this thesis to find the accuracy of the results of the algorithm [12].

The second quantized Hamiltonian of the static water molecule generally is of the form [1]:

$$H = \sum_{i,j=1}^{12} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{12} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l,$$

where a_i^\dagger and a_j are the fermionic creation and annihilation operators and h is the respective interaction coefficient. In the ground state, we can assume that the two uppermost orbitals of the

oxygen atom are unoccupied. In that case, 12 spin-orbitals have to be taken in consideration and the Hamiltonian is a sum over each one of these spin states. Bian et al. [1] reduce this Hamiltonian, using parity transformations and simplifications to the following form:

$$H = \sum_{i=j}^N \alpha_j P_j$$

Here, α_j is a function of the hydrogen-hydrogen bond length, and P_j is a multi-qubit Pauli operator, a tensor product of the four Pauli operators which are defined as the following [7]:

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

An example of a multi-qubit Pauli operator would then be:

$$P = Z \otimes X.$$

The Hamiltonian consists of a sum of up to N terms, where in this case $N = 2^4 = 16$, equal to the number of possible multi-qubit operators. Once the Hamiltonian is reduced, the ground energy can be derived from the Hamiltonian. There are several well-established algorithms. Bian et al. [1] compare five methods for calculating the ground-state energy of the water molecule, namely:

- *Trotter Phase Estimation Algorithm*
This method uses Trotter-Suzuki decomposition to approximate the propagating term $e^{-i\alpha_i h_i t}$, and subsequently extracts the ground state energy from the phase. The Trotter PEA requires $\mathcal{O}(n)$ qubits to run and has a gate complexity of $\mathcal{O}(\frac{n^5}{(\epsilon/A)^2})$, where n is the number of orbital basis functions, $A = \sum_{i=1}^L |\alpha_i|$ and ϵ is the desired accuracy of the energy.
- *Direct Implementation of Hamiltonian in First Order*
This method largely relies on the same principles as the Trotter PEA, but it employs a different unitary operator U . This Direct-PEA requires $\mathcal{O}(n)$ qubits to run and has a gate complexity of $\mathcal{O}(\frac{n^5}{(\epsilon/A)^2})$.
- *Direct Implementation of Hamiltonian in Second Order*
This method is the same as the First Order Direct-PEA, but it approximates U to the second order instead. This variant of the Direct-PEA requires $\mathcal{O}(n)$ qubits to run and has a gate complexity of $\mathcal{O}(\frac{n^5}{(\epsilon/A)^{1.3}})$.
- *Direct Measurement of Hamiltonian*
This method translates the Hamiltonian directly into a quantum circuit and retrieves the ground energy by repeatedly measuring. Direct measurement requires $\mathcal{O}(n)$ qubits to run and has a gate complexity of $\mathcal{O}(n^5)$.
- *Variational Quantum Eigensolver*
The VQE prepares a trial wave function and approximates the energy by iteratively retrieving the Pauli operator tensor products. This algorithm is often used on hybrid computers, as the optimization algorithms required are much faster on a classical computer than a quantum computer. The VQE only requires n qubits to run, and has a gate complexity of $\mathcal{O}(n^2 d)$, where d is the number of iterations of entangling gates.

According to Bian et al. [1], it is evident that all five methods are viable options for solving the ground energy problem. There are however some major variations regarding gate complexity and qubit number. Second order Direct-PEA has the best gate complexity, but the VQE seems to be the most practical method for the near future, as it has decently efficient gate computations and, most importantly, requires the least amount of qubits.

$$(I - 2|\beta\rangle\langle\beta|) \otimes I = \sum_j |j\rangle\langle j| \otimes P_j$$

The number of possible methods for the ground state problem are obviously not limited to the aforementioned five. Poulin et al. [8] recently proposed another method named Spectrum by Quantum Walk, which bypasses the need to approximate the time-evolution operator, by initializing the quantum computer to an invariant subspace of the unitary operator. Doing so allows you to use any unitary operator which is a function of the Hamiltonian. Poulin et al. [8] offer a specific unitary operator which, when initialized in the right bases, can be precisely implemented, avoiding any errors that might come with Trotter or Taylor approximations. Currently, no research has applied the Spectrum by Quantum Walk algorithm to the water molecule.

2.1 Methodology

The research process of this capstone will be composed of three main components. The first component consists of a literature review on the fundamentals on quantum computing, introducing standard conventions and treating concepts appearing frequently in later sections. To do so, several established texts such as Nielsen and Chuang [6], Steane [13] and Divincenzo [4] will be synthesised. The second component expands on and provides context for the algorithm proposed by Poulin et al. [8], and it will also elucidate the relevant atomic structure of the water molecule in the form of a literature review. Furthermore, this part will also cover the implementation of the algorithm into a quantum circuit using Cirq¹, Google’s open-source Python-based quantum computing package. The final part of this thesis will apply the quantum circuit of the algorithm to the specific Hamiltonian of the water molecule, retrieving the eigenstates of the Hamiltonian. Ultimately, this paper aims to develop an order of gate complexity as to compare the efficiency of the quantum walk algorithm to the five methods presented by Poulin et al. [8].

2.1.1 Quantummechanical foundations

Before we delve into the specifics of quantummechanics, a basic understanding of the quantummechanical principles governing qubits is needed. The state of some general quantummechanical system is described by its wavefunction, ϕ . A time-independent wavefunction is often expressed as some linear combination of orthonormal basis states, such that.

However, as the natural language of quantum mechanics is linear algebra, it is commonpractice to describe states in bra-ket notation (Source). States are described as vectors, and the simplest arbitrary quantummechanical system can be written:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

where ψ has to satisfy the normalization condition, implying that $\alpha^2 + \beta^2 = 1$. This system is called the *qubit*, which lives in a two-dimensional Hilbert space. The defining feature of qubits is that they are in quantum superposition. When measuring a qubit, the outcome of the measurement in the so-called computational basis will still be either $|0\rangle$ or $|1\rangle$, but these outcomes occur with probabilities depending on the superposition of the state, namely $|\alpha|$ or $|\beta|$. Applying quantum logic gates manipulates both basis states at the same time, resulting in an increased computational potential when compared to classical bits. The orthonormal basis states $|0\rangle$ and $|1\rangle$ are generally just an abstract representation of a two-level system, but depending on the type of quantum computer, they can be represented physical properties such as spin in quantum dots as well as energy levels in trapped ions [mcardle].

Whenever there is a system with n qubits, the joint state of that system is described by taking the tensor product of each individual state of that system. Taking a tensor product of two states is

¹<https://github.com/quantumlib/Cirq>

mathematically equivalent to taking the Kronecker product of the vectors of that state. For some arbitrary states $|\phi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ and $|\psi\rangle = \begin{pmatrix} \gamma \\ \delta \end{pmatrix}$, the joint state is given by

$$|\phi\rangle \otimes |\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \otimes \begin{pmatrix} \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} \alpha\gamma \\ \alpha\delta \\ \beta\gamma \\ \beta\delta \end{pmatrix}$$

FOUR POSTULATES, SEE SHOR

2.1.2 Simulation

The core objective of simulation is solving the set of differential equations that describe the physical evolution in time of that system. In the case of quantum simulation, the dynamical behaviour of the system is described by the Schrödinger equation,

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle.$$

Quantum simulation is “DIFFICULT” as the number of differential equation grows exponentially with the number of qubits that are evolving, as one qubit requires two differential equations to be solved.

Quantum simulation can be divided into two different sets of problems, the dynamic problem and the static problem. The static problem consists of preparing the (correct) initial state and the dynamical problem consists of reproducing how the time-evolution unitary operator, $U = \exp\{-iHt\}$ affects the state of the system.

The initial idea that motivated the entire field of quantum simulation, is that the storage needed to describe the wavefunction of a system of N particles grows with $\mathcal{O}(\exp(N))$ on a classical computer, while this relation is $\mathcal{O}(N)$ for qubits [2]. However, one cannot simply retrieve obtain a useful description of the wavefunction stored in qubits, as a classical representation of the wavefunction requires repeated measurements which, due to the collapse of the state during measurements, is a futile process. Instead, alternative processes, such as finding expectation values of observables, have to be utilized. Another important condition that has been satisfied, is that evolving the wavefunction in time is efficiently possible for Hamiltonians that are to a large extent physically realizable [2]. That is to say that the number of gates needed to simulate a system grows polynomially, rather than exponentially with parameters such as system size and time.

Furthermore, it is important to note that essentially all algorithms within quantum chemistry assume error-free quantum computations. At this point in time, fully coherent quantum computation has not yet been realized, as in the physical realizations of quantum computers today are still too error prone. The process of minimizing decoherence in quantum computers is highly instrumental to quantum computing and is an entire own subfield of quantum computing (Quantum Error Correction), which is out of scope for present research. We refer interested readers to the book Quantum Computation and Quantum Information by Nielsen and Chuang [6] for more information. The fact that quantum chemistry algorithms don't account for errors mean that none of these algorithms are executable in a non-trivial way yet i.e. deliver results that classical computers couldn't have obtained. This doesn't mean that these algorithms cannot be implemented, as we will see a rudimentary implementation of a specific quantum simulation algorithm later.

is this out of place?

Hamiltonian simulation roughly correlates to the time-dependent part of simulation as outlined before Different models of systems place different constraints on the manifestation of the form of the Hamiltonian. For most physical systems of n particles the Hamiltonian can be written as $H = \sum_k^L H_k$ where each H_k acts on a specific subsystem. Often these terms are two-body interaction terms such as $X_i X_j$ or even one-body Hamiltonians X_i . More specifically, the spin Ising model $H_{\text{Ising}} = g \sum_j X_j + J \sum_{\langle i,j \rangle} Z_i Z_j$ consists entirely of a linear combination of such interaction terms. The conventional method for simulating Hamiltonians of such form is to approximate the

make nice transition

time-evolution operator such that

$$U(t) \approx \left(e^{-iH_1 t/n} \dots e^{-iH_\ell t/n} \right)^n$$

. The method for approximating U as such is called *Trotter decomposition*, and as the gatecount grows polynomially with the number of qubits and time, this method is efficient for local-interaction Hamiltonians [2].

However, not all Hamiltonians satisfy the local-interaction condition of the Trotter decomposition, such as the electronic structure problem. The Hamiltonian of the electronic structure problem of K nuclei and N electrons is the following [5]:

$$H = - \sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_I \frac{\hbar^2}{2M_I} \nabla_I^2 - \sum_{i,I} \frac{e^2}{4\pi\epsilon_0} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2} \sum_{I \neq J} \frac{e^2}{4\pi\epsilon_0} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|}.$$

Here, M_I , \mathbf{R}_I , and Z_I represent respectively the mass, the position, and the atomic number of the I th nucleus. \mathbf{r}_i represents the position of the i -th electron. Since a nucleus is many times heavier than an electron we can utilise the Born-Oppenheimer approximation, neglecting the electron's position and treating the nuclei as classical point charges [5]. The approximated Hamiltonian becomes:

$$H_e = - \sum_i \frac{\nabla_i^2}{2} - \sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

This Hamiltonian however is in its current form still of little use from a quantum computing perspective, as we cannot translate this to qubits. Therefore we now write this Hamiltonian in the second quantization formalism of Quantum Field Theory. An in-depth explanation of the quantisation formalism is out of scope for this research, but the rough idea of second quantisation is that *fields* are being quantised rather than variables. The second quantised form of the electronic Hamiltonian corresponds to the following.

$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

where

$$h_{pq} = \int d\mathbf{x} \phi_p^*(\mathbf{x}) \left(-\frac{\nabla^2}{2} - \sum_I \frac{Z_I}{|\mathbf{r} - \mathbf{R}_I|} \right) \phi_q(\mathbf{x})$$

$$h_{pqrs} = \int d\mathbf{x}_1 d\mathbf{x}_2 \frac{\phi_p^*(\mathbf{x}_1) \phi_q^*(\mathbf{x}_2) \phi_r(\mathbf{x}_2) \phi_s(\mathbf{x}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

a_p^\dagger and a_q are respectively the fermionic creation and annihilation operators. These operators excite or de-excite electrons into spin-orbitals, and obey the following anti-commutation relations

$$\{a_p, a_q^\dagger\} = a_p a_q^\dagger + a_q^\dagger a_p = \delta_{pq}.$$

$$\{a_p, a_q\} = \{a_p^\dagger, a_q^\dagger\} = 0$$

To simulate the electronic structure problem in its second quantized form, a map from operators acting on indistinguishable fermions to operators acting on distinguishable qubits is needed [5]. There are several methods of implementing this map, such as the Jordan Wigner transformation and the Bravyi-Kitaev encoding.

The Jordan-Wigner transformation writes the annihilation and creation operators in terms of Pauli matrices, such that [3]

$$a_j \rightarrow I^{\otimes n-j-1} \otimes \sigma_+ \otimes \sigma_z^{\otimes j}, \text{ and } a_j^\dagger \rightarrow I^{\otimes n-j-1} \otimes \sigma_- \otimes \sigma_z^{\otimes j}$$

$$\sigma_+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \sigma_- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

The Bravyi-Kitaev expression for the operators in terms of Pauli matrices is significantly more involved than the respective Jordan-Wigner expression, and can be found in [10]. Applying any of these two encodings to the second quantised Hamiltonian of the H_2 molecule will result in the following representation:

$$\begin{aligned} \hat{H}_{BK} = & -0.812611 + 0.171201\sigma_0^z + 0.16862325\sigma_1^z - 0.2227965\sigma_2^z + 0.171201\sigma_1^z\sigma_0^z \\ & + 0.12054625\sigma_2^z\sigma_0^z + 0.17434925\sigma_3^z\sigma_1^z + 0.04532175\sigma_2^x\sigma_1^z\sigma_0^x + 0.04532175\sigma_2^y\sigma_1^z\sigma_0^y \\ & + 0.165868\sigma_2^z\sigma_1^z\sigma_0^z + 0.12054625\sigma_3^z\sigma_2^z\sigma_0^z - 0.2227965\sigma_3^z\sigma_2^z\sigma_1^z \\ & + 0.04532175\sigma_3^z\sigma_2^x\sigma_1^z\sigma_0^x + 0.04532175\sigma_3^y\sigma_2^z\sigma_1^z\sigma_0^y + 0.165868\sigma_3^z\sigma_2^z\sigma_1^z\sigma_0^z \end{aligned}$$

This Hamiltonian is well suited to quantum computers as it will amount to one 8×8 matrix acting on a four-qubit state.

2.1.3 State preparation and the quantum Zeno effect

Any quantum algorithm for ground state energy estimation, such as the one discussed in this research, requires (eigen)state preparation, as $H_k|\psi\rangle = E_k|\psi\rangle$ only when H is acting on an eigenstate. In the Spectrum by Quantum Walk algorithm, phase estimation performed as a projective energy measurement [Poulin]. Then it follows that for some approximation of the eigenstate $|\tilde{\phi}\rangle$,

the state of the system collapses to the actual ground state $|\phi\rangle$ with probability $|\langle\tilde{\phi}|\phi\rangle|^2$. Depending on the form of the Hamiltonian, obtaining $|\tilde{\phi}\rangle$ can be a difficult task. Poulin et al. [8] offer a method for obtaining this approximation, which is rather similar to the adiabatic state preparation.

The state preparation sequence of poulin goes as follows. We define the Hamiltonian to be a composite sum of a simpler Hamiltonian H_0 and some other interaction term V . This simpler Hamiltonian H_0 is one we know the ground state of. When considering the electronic structure problem of H_2 , an example for H_0 could be the transverse field Ising model. We can then rewrite the Hamiltonian as a function of some parameter g , where V is linearly related to g :

$$H = H_0 + gV$$

We are now able to prepare the physical register of our quantum computer in the simpler ground state $H = |\phi(g=0)\rangle$. Then we perform a sequence of energy measurements where we increase g slightly for each measurement. Ultimately, if the increments of g are sufficiently small, performing the energy measurement of $H(g=1)$ will result in the wave function collapsing to $|\phi(g=1)\rangle$, which is the actual ground state of the system we are simulating.

finish section

2.1.4 Nomenclature and important identities

In this chapter, the Spectrum by Quantum Walk algorithm, proposed by Poulin et al. [8], is discussed. Before this algorithm is examined in further detail, the following small section is dedicated to remove any confusion about conventions or identities used later on.

Within quantum computing, j represents a binary bit string. In present thesis, a four-qubit system is considered, so for consistency's sake all bit strings are expressed in the four-bit basis. For

example, the bit-string of eleven is represented in vector form by the following:

$$|11\rangle = |1011\rangle = |1\rangle \otimes |0\rangle \otimes |1\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Or generally, some state $|n\rangle$ in \mathbb{R}^{16} can be represented by $\{e_{n+1} \mid 1 \leq n+1 \leq 16\}$, where e_{n+1} is a vector with a 1 inserted at the $n+1^{th}$ position, and 0's elsewhere.

All bit string states are orthogonal, implying

$$\langle i|j\rangle = \delta_{i,j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}.$$

As for the outer product,

$$|i\rangle\langle j| = \delta_{i,j} e_{i+1,j+1}$$

When summing bit string outer products over the n -dimensional space, each basis vector in \mathbb{R}^n has a contribution of 1, resulting in an n by n matrix with only entries of 1 on the diagonal, which is the identity matrix:

$$\sum_j^n |j\rangle\langle j| = I_n$$

The expectation value of some observable \mathbb{A} measured in some basis $\{\varphi, \phi\}$ is:

$$\langle \varphi | \mathbb{A} | \phi \rangle = \langle \varphi | \mathbb{A} \phi \rangle = \langle \mathbb{A}^\dagger \varphi | \phi \rangle$$

However, if \mathfrak{c} is some scalar, then:

$$\langle \varphi | \mathfrak{c} | \phi \rangle = \langle \varphi | \mathfrak{c} \phi \rangle = \mathfrak{c} \langle \varphi | \phi \rangle$$

An important tensor product identity is the following:

$$(U \otimes V)(|\psi\rangle \otimes |\phi\rangle) = (U|\psi\rangle) \otimes (V|\phi\rangle)$$

2.1.5 Postulate of Operators

The goal of this algorithm, and of many other quantum simulation algorithms, is to obtain expectation values of the eigenstates of the Hamiltonian of the system. However, while many other algorithms aim to reproduce the dynamics of a quantum system by approximating the time evolution operator, this algorithm aims to find a useful initial state, which is often the ground state of the

Hamiltonian. As the Hamiltonian is absolutely fundamental to this method, let us define this first. First we have to assume that the Hamiltonian can be written in the form

$$H = \sum_{j=0}^N \alpha_j P_j,$$

where j represents some possible state of the system. In the case of a simple molecule, this state would align with the occupancy of certain (spin-)orbitals. We sum these states up to N , which is the number of possible states (in the case of a molecule, the number of possible orbital combinations). P_j here is a multi-qubit Pauli operator, a tensor product of the four Pauli operators which are defined as the following [6]:

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

Before we move forward, we must ensure that the Hamiltonian we are working with has mathematically desirable properties, such as normalization. We do so by introducing a scaling factor of $\mathcal{N} = \sum_{j=0}^N |\alpha_j|$ [8].

Then our new, rescaled Hamiltonian which we will call \bar{H} , takes the following form:

$$\bar{H} = \frac{H}{\mathcal{N}} = \sum_j |\beta_j|^2 P_j, \quad (2.1)$$

where $\beta_j = \sqrt{|\alpha_j|/\mathcal{N}}$. Due to the nature of the scaling factor \mathcal{N} , $\sum_j |\beta_j|^2 = 1$. Poulin et al. [8] define β, B, S and V as following:

$$\begin{aligned} |\beta\rangle &= B |0\rangle = \sum_j \beta_j |j\rangle \\ S &= (B(I - 2|0\rangle\langle 0|)B^\dagger) \otimes I = (I - 2|\beta\rangle\langle\beta|) \otimes I \\ V &= \sum_j |j\rangle\langle j| \otimes P_j \end{aligned}$$

It will be useful to check if S and V are unitary, so for S we multiply it with its complex conjugate, which, since S is not complex, is the same as taking the square:

$$\begin{aligned} SS^* &= S^2 = ((I - 2|\beta\rangle\langle\beta|) \otimes I)((I - 2|\beta\rangle\langle\beta|) \otimes I) \\ &= (I - 2|\beta\rangle\langle\beta|)(I - 2|\beta\rangle\langle\beta|) \otimes I^2 \\ &= I^2 - 2I|\beta\rangle\langle\beta| - 2|\beta\rangle\langle\beta|I + 4|\beta\rangle\langle\beta|\langle\beta|\beta\rangle \\ &= I^2 - 4|\beta\rangle\langle\beta| + 4|\beta\rangle\langle\beta| = I^2 = I \end{aligned}$$

Same process for the operator V :

²The outer product of a vector only produces elements on the diagonal, so multiplying with identity returns that same outer product

prove
they're Her-
mitian

$$\begin{aligned}
VV^* &= V^2 = \sum_j |j\rangle\langle j| \otimes P_j \cdot \sum_k |k\rangle\langle k| \otimes P_k \\
&= \sum_j \sum_k |j\rangle\langle j|k\rangle\langle k| \otimes P_j P_k \\
&= \sum_j \sum_k \delta_{j,k} |j\rangle\langle j| \otimes P_j P_k \\
&= \sum_j |j\rangle\langle j| \otimes P_j P_j
\end{aligned}$$

$$\begin{aligned}
&\text{As } \sum_j^n |j\rangle\langle j| = I_n, \\
&V^2 = I
\end{aligned}$$

2.1.6 Orthonormal bases

This algorithm relies on one fundamental property, namely that “there exists an invariant subspace of W on which the spectrum of W is the simple function of H ” (The operator W will be defined in a later stage). This statement implies that there is such W , where because it is a function of the Hamiltonian in a certain subspace, we can retrieve properties of that Hamiltonian from the operator W . Poulin et al. [8] postulate the following orthonormal basis, in which S and V preserve the substate spanned by those basis, which will be the same substate that W will be initialized to:

$$|\varphi_k^0\rangle = \sum_j \beta_j |j\rangle \otimes |\phi_k\rangle \quad (2.2)$$

$$|\varphi_k^1\rangle = \frac{1}{\sqrt{1 - E_k^2}} (V - E_k) |\varphi_k^0\rangle, \quad (2.3)$$

Here, k is a measure of the state of the eigenfunctions of the hamiltonian. When $k = 0$, we are working with the ground-state. the place on the Let us prove that φ_k^0 and φ_k^1 are normalized and orthogonal:

$$\langle \varphi_k^0 | \varphi_k^0 \rangle = (\langle \beta | \otimes \langle \phi_k |) (|\beta\rangle \otimes |\phi_k\rangle) \quad (2.4)$$

$$= \langle \beta | \beta \rangle \otimes \langle \phi_k | \phi_k \rangle \quad (2.5)$$

$$= 1 \quad (2.6)$$

$$\begin{aligned}
\langle \varphi_k^1 | \varphi_k^1 \rangle &= \langle \varphi_k^0 | \frac{1}{\sqrt{1 - E_k^2}} (V - E_k) \frac{1}{\sqrt{1 - E_k^2}} (V - E_k) | \varphi_k^0 \rangle \\
&= \langle \varphi_k^0 | \frac{1}{1 - E_k^2} (V - E_k)^2 | \varphi_k^0 \rangle \\
&= \frac{1}{1 - E_k^2} \langle \varphi_k^0 | (V^2 - 2E_k V + E_k^2) | \varphi_k^0 \rangle \\
&= \frac{1}{1 - E_k^2} \langle \varphi_k^0 | (I - 2E_k V + E_k^2) | \varphi_k^0 \rangle
\end{aligned}$$

As the following identity will appear often, a separate definition is made .

$$\begin{aligned}
\langle \varphi_k^0 | V | \varphi_k^0 \rangle &= \langle \varphi_k^0 | \left(\sum_j |j\rangle \langle j| \otimes P_j \right) \sum_l \beta_l |l\rangle \otimes |\phi_k^0\rangle \\
&= \langle \varphi_k^0 | \sum_j \sum_l \beta_l |j\rangle \langle j|l\rangle \otimes P_j | \phi_k^0 \rangle \\
&= \left(\sum_m \beta_m^* \langle m | \otimes \langle \phi_k | \right) \sum_j \sum_l \beta_l |j\rangle \delta_{j,l} \otimes P_j | \phi_k \rangle \\
&= \sum_m \sum_j \beta_m^* \beta_j \langle m | j \rangle \otimes \langle \phi_k | P_j \phi_k \rangle \\
&= \sum_m \sum_j \beta_m^* \beta_j \delta_{m,j} \otimes \langle \phi_k | P_j \phi_k \rangle \\
&= \sum_j |\beta_j|^2 \langle \phi_k | P_j \phi_k \rangle \\
&= \sum_j \left\langle \phi_k \left| |\beta_j|^2 P_j \phi_k \right. \right\rangle
\end{aligned}$$

As $\bar{H} | \phi_k \rangle = E_k | \phi_k \rangle$ and $\bar{H} = \sum_j |\beta_j|^2 P_j$,

$$\langle \varphi_k^0 | V | \varphi_k^0 \rangle = \langle \phi_k | E_k \phi_k \rangle = E_k \quad (2.7)$$

Continuing proof of orthonormality of φ_k^1 using equation 4:

$$\begin{aligned}
\langle \varphi_k^1 | \varphi_k^1 \rangle &= \frac{1}{1 - E_k^2} \langle \varphi_k^0 | (I - 2E_k V + E_k^2) | \varphi_k^0 \rangle \\
&= \frac{1}{1 - E_k^2} \langle \varphi_k^0 | (I - 2E_k^2 + E_k^2) | \varphi_k^0 \rangle \\
&= \frac{1}{1 - E_k^2} \langle \varphi_k^0 | (I - E_k^2) | \varphi_k^0 \rangle \\
&= \frac{1 - E_k^2}{1 - E_k^2} \langle \varphi_k^0 | \varphi_k^0 \rangle \\
&= 1
\end{aligned}$$

Proof of orthogonality, using equation 4

$$\begin{aligned}
\langle \varphi_k^0 | \varphi_k^1 \rangle &= \langle \varphi_k^0 | \frac{1}{\sqrt{1 - E_k^2}} (V - E_k) | \varphi_k^0 \rangle \\
&= \langle \varphi_k^0 | \frac{1}{\sqrt{1 - E_k^2}} (E_k - E_k) | \varphi_k^0 \rangle \\
&= 0
\end{aligned}$$

2.1.7 Blockdiagonality

Poulin et al [8] state that the unitary property of S and V allow them to be put in block diagonal form with 2×2 blocks. A general block diagonal matrix only has nonzero entries in the blocks of size $n \times n$ on the diagonal, which for $n = 2$ looks like the following:

$$\left(\begin{array}{cc|cc} a & b & 0 & 0 \\ c & d & 0 & 0 \\ \hline 0 & 0 & a & b \\ 0 & 0 & c & d \end{array} \right)$$

We can put the expectation values of S and V in one of such matrices in the subspace of φ_k^0 and φ_k^1 . The matrix with placeholder values then looks like the following:

$$\begin{array}{c|cc|cc|c|cc}
 & |\varphi_0^0\rangle & |\varphi_0^1\rangle & |\varphi_1^0\rangle & |\varphi_1^1\rangle & \dots & |\varphi_k^0\rangle & |\varphi_k^1\rangle \\
 \hline
 \langle\varphi_0^0| & V_{11} & V_{21} & 0 & 0 & & 0 & 0 \\
 \langle\varphi_0^1| & V_{12} & V_{22} & 0 & 0 & & 0 & 0 \\
 \hline
 \langle\varphi_1^0| & 0 & 0 & V_{33} & V_{43} & & 0 & 0 \\
 \langle\varphi_1^1| & 0 & 0 & V_{43} & V_{44} & & 0 & 0 \\
 \hline
 \vdots & & & & & \ddots & & \\
 \hline
 \langle\varphi_k^0| & 0 & 0 & 0 & 0 & & a & b \\
 \langle\varphi_k^1| & 0 & 0 & 0 & 0 & & c & d
 \end{array} \quad (2.8)$$

The off-diagonal elements are zero as $\langle\phi_k|\phi_l\rangle = \delta_{k,l}$. In other words, all the eigenstates of the Hamiltonian are orthogonal. We can find the values of S and V in the basis by

$$\begin{aligned}
 \langle\varphi_0^0| S |\varphi_0^0\rangle &= \langle\varphi_0^0| (I - 2|\beta\rangle\langle\beta|) \otimes I |\varphi_0^0\rangle \\
 &= \langle\varphi_0^0| ((I - 2|\beta\rangle\langle\beta|) \otimes I) \sum_j \beta_j |j\rangle \otimes |\phi_0\rangle \\
 &= \langle\varphi_0^0| \sum_j (I - 2|\beta\rangle\langle\beta|) \beta_j |j\rangle \otimes |\phi_0\rangle \\
 &= \langle\varphi_0^0| - |\beta\rangle \otimes |\phi_0\rangle \\
 &= -(\langle\beta| \otimes \langle\phi_0|) |\beta\rangle \otimes |\phi_0\rangle \\
 &= -1
 \end{aligned}$$

Before we find the value of $\langle\varphi_0^1| S |\varphi_0^1\rangle$, let us find what applying S and V in succession on a general state results:

$$\begin{aligned}
 SV &= ((I - 2|\beta\rangle\langle\beta|) \otimes I) \sum_j |j\rangle\langle j| \otimes P_j \\
 &= ((I - 2|\beta\rangle\langle\beta|) \sum_j |j\rangle\langle j|) \otimes IP_j \\
 &= \sum_j ((I - 2|\beta_j|^2 |j\rangle\langle j|) |j\rangle\langle j|) \otimes P_j \\
 &= \sum_j (|j\rangle\langle j| - 2|j\rangle\langle j| |j\rangle\langle j|) \otimes P_j \\
 &= - \sum_j |j\rangle\langle j| \otimes P_j \\
 &= -V
 \end{aligned}$$

As S is a reflexion operator, the result makes sense, since V also preserves the subspace spanned by the orthonormal bases. Let us finish filling out the block diagonal matrix of S , by finding the remaining values.

$$\begin{aligned}
\langle \varphi_0^1 | S | \varphi_0^1 \rangle &= \langle \varphi_0^1 | ((I - 2|\beta\rangle\langle\beta|) \otimes I) \frac{1}{\sqrt{1-E_0^2}} (V - E_0) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^1 | \frac{1}{\sqrt{1-E_0^2}} (-V + E_0) (-| \varphi_0^0 \rangle) \\
&= \langle \varphi_0^0 | \frac{1}{\sqrt{1-E_0^2}} (V - E_0) \frac{1}{\sqrt{1-E_0^2}} (-V + E_0) - (| \varphi_0^0 \rangle) \\
&= -\langle \varphi_0^0 | \frac{1}{1-E_0^2} (-V^2 + E_0V + E_0V - E_0^2) | \varphi_0^0 \rangle
\end{aligned}$$

As $\langle \varphi_k^0 | V | \varphi_k^0 \rangle = E_k$,

$$\begin{aligned}
\langle \varphi_0^1 | S | \varphi_0^1 \rangle &= -\langle \varphi_0^0 | \frac{1}{1-E_0^2} (-1 + E_0^2) | \varphi_0^0 \rangle \\
&= -\langle \varphi_0^0 | \frac{-(1-E_0^2)}{1-E_0^2} | \varphi_0^0 \rangle \\
&= -\langle \varphi_0^0 | (-| \varphi_0^0 \rangle) \\
&= \langle \varphi_0^0 | \varphi_0^0 \rangle \\
&= 1
\end{aligned}$$

$$\begin{aligned}
\langle \varphi_0^0 | S | \varphi_0^1 \rangle &= \langle \varphi_0^0 | ((I - 2|\beta\rangle\langle\beta|) \otimes I) \frac{1}{\sqrt{1-E_0^2}} (V - E_0) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^0 | \frac{1}{\sqrt{1-E_0^2}} (-V + E_0) | -\varphi_0^0 \rangle \\
&= -\langle \varphi_0^1 | \frac{1}{\sqrt{1-E_0^2}} (-E_0 + E_0) | \varphi_0^0 \rangle \\
&= -\langle \varphi_0^1 | 0 | \varphi_0^0 \rangle \\
&= 0
\end{aligned}$$

As the operator S is symmetric around the diagonal, S is self adjoint and from the identity

$$\langle \psi | A^\dagger | \phi \rangle = \langle \phi | A | \psi \rangle^*$$

we can conclude that $\langle \varphi_0^0 | S | \varphi_0^1 \rangle = \langle \varphi_0^1 | S | \varphi_0^0 \rangle = 0$.

The block of S is now completed, and looks like the following:

$$S = \begin{matrix} & \begin{matrix} | \varphi_0^0 \rangle & | \varphi_0^1 \rangle \end{matrix} \\ \begin{matrix} \langle \varphi_0^0 | \\ \langle \varphi_0^1 | \end{matrix} & \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \end{matrix} \quad (2.9)$$

From these values, it is clear that there is no k -dependency and therefore above matrix can be generalised for all k -values. The entirety of matrix 4 can be condensed into the following:

$$S = \begin{matrix} & \begin{matrix} | \varphi_k^0 \rangle & | \varphi_k^1 \rangle \end{matrix} \\ \begin{matrix} \langle \varphi_k^0 | \\ \langle \varphi_k^1 | \end{matrix} & \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \end{matrix} \quad (2.10)$$

Let us find the equivalent matrix for the operator V. In equation 4, it has been shown that $\langle \varphi_k^0 | V | \varphi_k^0 \rangle = E_k$. Moving on,

$$\begin{aligned}
\langle \varphi_0^0 | V | \varphi_0^1 \rangle &= \langle \varphi_0^0 | \frac{1}{\sqrt{1-E_0^2}} (V^2 - E_0 V) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^0 | \frac{1}{\sqrt{1-E_0^2}} (1 - E_0^2) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^0 | \sqrt{1-E_0^2} | \varphi_0^0 \rangle \\
&= \sqrt{1-E_0^2} \langle \varphi_0^0 | \varphi_0^0 \rangle \\
&= \sqrt{1-E_0^2}
\end{aligned}$$

As V is also symmetric and therefore self-adjoint,

$$\langle \psi | A^\dagger | \phi \rangle = \langle \phi | A | \psi \rangle^*$$

holds again and thus

$$\langle \varphi_0^0 | V | \varphi_0^1 \rangle = \langle \varphi_0^1 | V | \varphi_0^0 \rangle = \sqrt{1-E_0^2}$$

Lastly, we need to find $\langle \varphi_0^1 | V | \varphi_0^1 \rangle$:

$$\begin{aligned}
\langle \varphi_0^1 | V | \varphi_0^1 \rangle &= \langle \varphi_0^1 | \frac{1}{\sqrt{1-E_0^2}} (V^2 - E_0 V) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^0 | \frac{1}{1-E_0^2} (V - E_0)(1 - E_0 V) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^0 | \frac{1}{1-E_0^2} (V - E_0 - E_0 + E_0^2 V) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^0 | \frac{1}{1-E_0^2} (-E_0 + E_0^3) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^0 | (-E_0 \frac{1-E_0^2}{1-E_0^2}) | \varphi_0^0 \rangle \\
&= \langle \varphi_0^0 | (-E_0) | \varphi_0^0 \rangle \\
&= -E_0
\end{aligned}$$

Once again, we can compile these value in the block matrix and generalize to any k -value in the range of energy states to obtain:

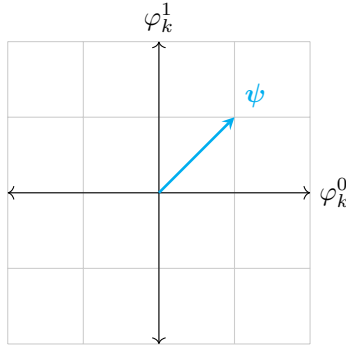
$$S = \begin{matrix} \langle \varphi_k^0 | \\ \langle \varphi_k^1 | \end{matrix} \begin{bmatrix} \frac{E_k}{\sqrt{1-E_0^2}} & \frac{\sqrt{1-E_0^2}}{-E_k} \end{bmatrix} \begin{matrix} | \varphi_k^0 \rangle \\ | \varphi_k^1 \rangle \end{matrix} \quad (2.11)$$

2.1.8 Creating the Unitary Walk Operator

Before we start thinking about constructing an operator from S and V , it is paramount to have a clear picture in mind of how S and V precisely act. In chapter 4.2 we have derived these operators in matrix form, in the subspace spanned by φ_k^0 and φ_k^1 .

Lets consider a general state in this subspace of the form $|\psi\rangle = c_0 |\varphi_k^0\rangle + c_1 |\varphi_k^1\rangle$, which would look like the following:

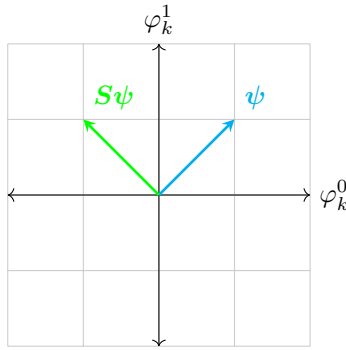
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Let us apply S to ψ :

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \begin{pmatrix} -c_0 \\ c_1 \end{pmatrix}$$

A visual representation of what happens when S is applied to ψ :



As is evident from the graph above, the S operator reflects any state in the subspace around the φ_k^1 axis. To see what effect V has on a state in this subspace, we can simply apply V to some state in the subspace. For efficiency reasons, we pick $c_0 = 1 \wedge c_1 = 0$.

$$\begin{aligned} V |\psi\rangle &= V |\varphi_k^0\rangle \\ &= \sum_j |j\rangle\langle j| \otimes P_j \sum_j \beta_j |j\rangle \otimes |\phi_0\rangle \\ &= \sum_j \beta_j |j\rangle \otimes P_j |\phi_k\rangle \end{aligned}$$

From this result, we conclude that V applies the specific Pauli operator, corresponding to the state of the system of qubits, to the k_{th} eigenstate of the Hamiltonian. Poulin et al. [8] define the unitary walk operator as:

$$W = S V e^{i\pi}$$

As W acts on the n system qubits and the $\log(N+1)$ ancillary registers, W is a $2^{n+\log(N+1)} \times$ $2^{n+\log(N+1)}$ matrix.

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2.2 Quantum Phase Estimation

The eigenvalues of all unitary operators, such as the unitary operator W , are unitary too and can be written in the form $\exp\{2\pi i\theta\}$.

2.2.1 Protocol

When implementing the Spectrum by Quantum Walk algorithm, the following general protocol is to be followed:

1. Normalize the Hamiltonian of the system to be simulated.
2. Create two registers: an ancillary register and a system register of sizes $\log(N)$ and n respectively.
3. Prepare an initial state of the form $B|0\rangle \otimes |\tilde{\phi}_0\rangle$.
4. Create an additional ancillary register of size t and perform phase estimation of W to obtain $|\theta_k\rangle$.
5. Repeat this process to find the normalized energy, as $\cos\theta_k = E_k$
6. Multiply E_k with N

identities:

$$\langle \varphi_k^\pm | \sigma | \varphi_k^\pm \rangle = \left(\frac{1}{\sqrt{2}} \langle \varphi_k^0 | \mp i \langle \varphi_k^1 | \right) \sigma \left(\frac{1}{\sqrt{2}} | \varphi_k^0 \rangle \pm i | \varphi_k^1 \rangle \right) \quad (2.12)$$

$$= \frac{1}{2} (\langle \varphi_k^0 | \sigma | \varphi_k^0 \rangle \pm i \langle \varphi_k^0 | \sigma | \varphi_k^1 \rangle \mp i \langle \varphi_k^1 | \sigma | \varphi_k^0 \rangle + \langle \varphi_k^1 | \sigma | \varphi_k^1 \rangle) \quad (2.13)$$

$$(2.14)$$

We now consider each term individually.

brackets fix

$$\begin{aligned} \langle \varphi_k^0 | \sigma | \varphi_k^0 \rangle &= \langle \beta | \otimes \langle \phi_k | \sigma | \beta \rangle \otimes | \phi_k \rangle \\ &= \langle \beta | \beta \rangle \otimes \langle \phi_k | \sigma | \phi_k \rangle \\ &= \langle \phi_k | \sigma | \phi_k \rangle \end{aligned}$$

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$$\begin{aligned} \langle \varphi_k^0 | \sigma | \varphi_k^1 \rangle &= \frac{1}{\sqrt{1-E_k^2}} \langle \beta | \otimes \langle \varphi_k | \sigma (V - E_k) | \beta \rangle \otimes | \phi_k \rangle \\ &= \frac{1}{\sqrt{1-E_k^2}} \langle \beta | \otimes \langle \varphi_k | \sigma \left(\sum_j \beta_j | j \rangle \otimes P_j | \phi_k \rangle - E_k | \beta \rangle \otimes | \phi_k \rangle \right) \\ &= \frac{1}{\sqrt{1-E_k^2}} \left(\sum_j |\beta_j|^2 \langle \phi_k | \sigma P_j | \phi_k \rangle - E_k \langle \phi_k | \sigma | \phi_k \rangle \right) \\ &= \frac{1}{\sqrt{1-E_k^2}} (E_k \langle \phi_k | \sigma | \phi_k \rangle - E_k \langle \phi_k | \sigma | \phi_k \rangle) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \langle \varphi_k^1 | \sigma | \varphi_k^0 \rangle &= (\langle \varphi_k^0 | \sigma | \varphi_k^1 \rangle)^* \\ &= 0 \end{aligned}$$

$$\langle \varphi_k^1 | \sigma | \varphi_k^1 \rangle = \frac{1}{1-E_k^2} \langle \varphi_k^0 | (V - E_k) \sigma (V - E_k) | \varphi_k^0 \rangle \quad (2.15)$$

$$= \frac{1}{1-E_k^2} \langle \varphi_k^0 | (V \sigma V - V \sigma E_k - E_k \sigma V + E_k \sigma E_k) | \varphi_k^0 \rangle \quad (2.16)$$

$$= \frac{1}{1-E_k^2} \langle \varphi_k^0 | V \sigma V | \varphi_k^0 \rangle - \langle \varphi_k^0 | V \sigma E_k | \varphi_k^0 \rangle \quad (2.17)$$

$$- \langle \varphi_k^0 | E_k \sigma V | \varphi_k^0 \rangle + \langle \varphi_k^0 | E_k \sigma E_k | \varphi_k^0 \rangle \quad (2.18)$$

We once again consider each expectation value individually.

$$\langle \varphi_k^0 | E_k \sigma E_k | \varphi_k^0 \rangle = E_k^2 \langle \phi_k | \sigma | \phi_k \rangle$$

Using equation 2.7, the following holds.

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$$\begin{aligned} \langle \varphi_k^0 | E_k \sigma V | \varphi_k^0 \rangle &= E_k \langle \varphi_k^0 | \sigma | \beta \rangle \otimes P_j | \phi_k \rangle \\ &= E_k \langle \beta | \beta \rangle \otimes \langle \phi_k | \sigma P_j | \phi_k \rangle \\ &= E_k \sum_j \langle \phi_k | \sigma | \beta_j \rangle^2 P_j | \phi_k \rangle \\ &= E_k^2 \langle \phi_k | \sigma | \phi_k \rangle \end{aligned}$$

As $\langle \varphi_k^0 | V \sigma E_k | \varphi_k^0 \rangle$ is symmetric to $\langle \varphi_k^0 | E_k \sigma V | \varphi_k^0 \rangle$, we can conclude that $\langle \varphi_k^0 | V \sigma E_k | \varphi_k^0 \rangle = E_k^2 \langle \phi_k | \sigma | \phi_k \rangle$

$$\begin{aligned}
\langle \varphi_k^0 | V \sigma V | \varphi_k^0 \rangle &= \langle \beta | \otimes \langle \phi_k | V \sigma V | \beta \rangle \otimes | \phi_k \rangle \\
&= \sum_l \langle l | \beta_l^\dagger \otimes \langle \phi_k | P_l \sigma \sum_j \beta_j | j \rangle \otimes P_j | \phi_k \rangle \\
&= \sum_j |\beta_j|^2 \langle j | j \rangle \otimes \langle \phi_k | P_j \sigma P_j | \phi_k \rangle \\
&= \sum_j |\beta_j|^2 \langle \phi_k | P_j \sigma P_j | \phi_k \rangle
\end{aligned}$$

We split this sum up into two separate sums, where an extra constraint is placed on the (anti)commutation relation of σ and P_j .

$$= \sum_{[\sigma, P_j=0]}^j |\beta_j|^2 \langle \phi_k | P_j \sigma P_j | \phi_k \rangle + \sum_{\{\sigma, P_j=0\}}^j |\beta_j|^2 \langle \phi_k | P_j \sigma P_j | \phi_k \rangle$$

In the sum where σ and P_j commute, we can switch the order of σ and P_j . We can do the same for the sum where σ and P_j commute, but that results in a sign change, as $AB = -BA$ for $\{A, B\} = 0$. This gives

$$= \sum_{[\sigma, P_j=0]}^j |\beta_j|^2 \langle \phi_k | P_j P_j \sigma | \phi_k \rangle - \sum_{\{\sigma, P_j=0\}}^j |\beta_j|^2 \langle \phi_k | P_j P_j \sigma | \phi_k \rangle.$$

As P_j is unconditionally unitary, $P_j^2 = 1$. We can now merge the two sums back together by defining an additional operator σ :

$$\sigma \star P_j = 0 \iff [\sigma, P_j] = 0 \wedge \sigma \star P_j = 1 \iff \{\sigma, P_j\} = 0.$$

Then the two sums can be written as

$$\sum_j |\beta_j|^2 (-1)^{\sigma \star P_j} \langle \phi_k | \sigma | \phi_k \rangle$$

Following the convention introduced by, we define another variable Γ :

$$\Gamma_\sigma = \sum_j |\beta_j|^2 (-1)^{\sigma \star P_j}$$

Then the expectation value can be written as

$$\langle \varphi_k^0 | V \sigma V | \varphi_k^0 \rangle = \Gamma_\sigma \langle \phi_k | \sigma | \phi_k \rangle \tag{2.19}$$

Filling in the individual expectation values in equation 2.17, we obtain

$$\begin{aligned}
\langle \varphi_k^1 | \sigma | \varphi_k^1 \rangle &= \frac{1}{1 - E_k^2} (\langle \varphi_k^0 | V \sigma V | \varphi_k^0 \rangle - \langle \varphi_k^0 | V \sigma E_k | \varphi_k^0 \rangle \\
&\quad - \langle \varphi_k^0 | E_k \sigma V | \varphi_k^0 \rangle + \langle \varphi_k^0 | E_k \sigma E_k | \varphi_k^0 \rangle) \\
&= \frac{\Gamma_\sigma - 2E_k^2 + E_k^2}{1 - E_k^2} \langle \phi_k | \sigma | \phi_k \rangle \\
&= \frac{\Gamma_\sigma - E_k^2}{1 - E_k^2} \langle \phi_k | \sigma | \phi_k \rangle.
\end{aligned}$$

We can now fill this expression back in equation 2.13 and obtain the value for the expectation value of some multi-qubit Pauli operator in the ϕ_k^\pm -basis.

$$\langle \varphi_k^\pm | \sigma | \varphi_k^\pm \rangle = \frac{1}{2} \left(1 + \frac{\Gamma_\sigma - E_k^2}{1 - E_k^2} \right) \langle \phi_k | \sigma | \phi_k \rangle$$

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