

## MAPPING FERMIONS TO QUBITS

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### 1 Introduction

"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy." - *Dr Richard Feynman* [1]

Ever since Dr Richard Feynman said these famous words at the end of his keynote speech in 1982, one of the main tasks facing quantum computers has been simulating quantum systems. Intuitively a quantum computer should be able to handle this problem better than a classic computer as they operate within the same bizarre world of entanglement and superposition. However, there are many challenges to overcome before quantum advantage can be achieved in this field. We will consider one such challenge in this essay: the optimum mapping scheme from fermions to qubits.

One of the most common classes of quantum systems we wish to simulate are those composed of fermions. In order to simulate these particles we must find a representation for them in terms a quantum computer can process, that is qubits and qubit operators. This poses a fundamental issue as fermions exhibit the non-local property of anti-commutation (**need to explain why it is non-local**), whereas qubits are independent local units. Therefore a non-trivial mapping scheme which introduces this non-local behaviour is necessary.

The first such mapping, the **Jordan-Wigner Transformation**, was invented nearly a century ago [2], and we will introduce it in Section 3. More recently, a number of new mappings have been developed including the **Bravyi-Kitaev map** and the **Derby-Klassen map**, which will be discussed in Section 4 and Section 5 respectively. Furthermore, recent research [3] has shown that the **fermionic enumeration** scheme used in a given mapping (we consider solely the Jordan-Wigner case) offers potential for increased locality with no additional

resources. This is elaborated on in Section 6.

It is important to consider how these mappings impact upon the fermionic simulation techniques used. Therefore, in Section 2 we will discuss how VQE and phase estimation can both be used to estimate the ground state energy of a system. Finally, in Section 7 we will compare the relative performance of these mappings in real-world applications (using simulated quantum computers).

**First and second quantisation - good pros v cons in vqe paper.** Grid vs Basis set look at Sam McArdles review

## 2 Applications to fermionic systems

### 2.1 Estimating ground state energies

Computing the ground state energy of a Hamiltonian is generally the first step in computing the energetic properties of molecules and materials [4]. Chemists have developed classical computational models for estimating the ground state, however, they all rely on approximations. Quantum computing opens up the potential for an exact (*full configuration interaction*) approach, which is unfeasible on a classical computer where it scales exponentially (**verify this is true**) in the number of fermionic modes.

#### 2.1.1 Variational Quantum Eigensolver

A VQE provides an upper bound on the ground state energy of a Hamiltonian by utilising the variational principle:

$$\frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \geq E_0 \quad \forall |\psi\rangle \in \mathcal{H} \quad (1)$$

The algorithm consists of two stages. First a variational ansatz is initialised based on a set of parameters  $\theta$ . Then, the Hamiltonian is measured a number of times, and the parameters of the ansatz are varied until a minimum is found. This is an example of a variational quantum algorithm, which performs a classical optimisation over a quantum oracle (**is this a correct description**). By exporting lots of the work to a classical computer, VQEs are one of the quantum algorithms that are achievable in the NISQ (Noisy Intermediate-scale Quantum) era.

The preparation of ansatz can be done without any regard for fermions or what underlying wavefunction it represents. Generally a given circuit structure is picked with some of the gates depending upon the parameters (i.e. an  $R_z(\theta)$  gate). However, there are some schemes for preparing ansatz that correlate to known wavefunctions, so the wavefunction corresponding to the minimum energy estimate can be found (**check this is true, find example and see if mapping is important** - Unitary Coupled Cluser - gaussian).

It is in the measurement of the Hamiltonian that the mapping becomes important. The Hamiltonian in question will be a combination of fermionic raising and lowering operators, so needs to be mapped to a combination of Pauli operators that can be measured on a quantum computer. **consider measurement strategies that minimise repetitions**. After this mapping has been performed we are left with a qubit Hamiltonian that is a sum of Pauli

strings (strings of Pauli operators). Therefore, we can measure the effectiveness of different mappings by the resource costs of implementing this qubit Hamiltonian. We will focus on three metrics (**this bit might be too similar to vqe page 31**):

- (i) **Number of qubits:** The less qubits required by the mapping the smaller the quantum computer required to run the simulation.
- (ii) **Average Pauli weight:** The average number of Pauli operators in each Pauli string in the Hamiltonian. The smaller the Pauli weight the less gates needed to measure the Hamiltonian, which reduces both the resource cost and the error due to gate infidelity.  
**Low-weight operators protect against barren plateau** doi:10.1038/s41467-021-21728-w.. **Could potentially elaborate here as it is a bit more complex than just less gates per string it also increases parallelisation and reduces ansatz depth. Mention locality**
- (iii) **Number of Pauli-strings:** Each Pauli-string is measured separately, so the fewer Pauli-strings to measure, the fewer times the ansatz needs to be initialized and measured.

### 2.1.2 Quantum Phase estimation

QPE can be used to estimate the energy levels of a Hamiltonian to  $n$  bits. This is achieved by applying successive steps of time evolution as a controlled gate with the target being the input state and the control being successive Hadamard ancilla qubits (illustrated in Fig. 1). Then by performing an inverse Quantum Fourier Transform on these ancilla qubits we get a superposition of binary expressions for the energy levels.

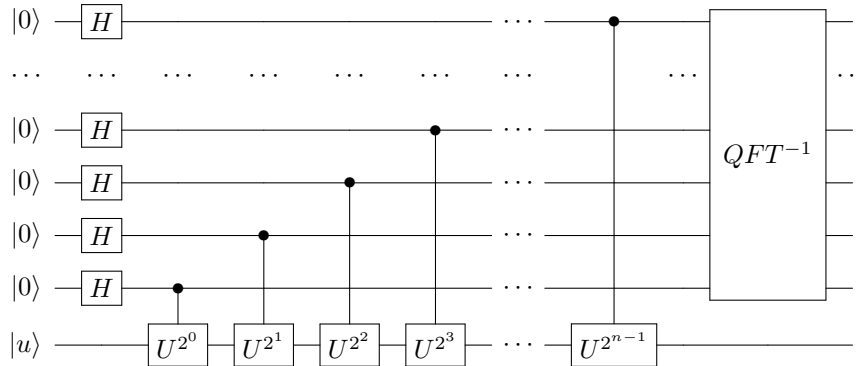


Fig. 1. Circuit diagram of QPE. In order to calculate energy levels  $U = e^{-2\pi i \hat{H}}$  is used.

An important feature of the algorithm is that the input state  $|u\rangle$  must have overlap with the ground state. This can be seen by working through in detail (we have adapted the following treatment from [5]):

- We can express  $|u\rangle$  in the basis of energy eigenstates:  $|u\rangle = \sum_i c_i |E_i\rangle$ . Therefore, the total state after the application of the Hadamard gates is:

$$\frac{1}{\sqrt{2^n}} \sum_i \sum_x |x\rangle c_i |E_i\rangle \quad (2)$$

- After the application of the controlled gates shown in Fig. 1, this transforms to:

$$\frac{1}{\sqrt{2^n}} \sum_i c_i (|0\rangle + e^{-2\pi i E_i 2^0} |1\rangle) (|0\rangle + e^{-2\pi i E_i 2^1} |1\rangle) \cdots (|0\rangle + e^{-2\pi i E_i 2^{n-1}} |1\rangle) |E_i\rangle \quad (3)$$

as  $x = x_0 2^0 + x_1 2^1 + \cdots + x_{n-1} 2^{n-1}$  for  $x_i \in \{0, 1\}$ , this reduces to:

$$\frac{1}{\sqrt{2^n}} \sum_i \sum_x e^{-2\pi i E_i x} c_i |x\rangle |E_i\rangle \quad (4)$$

- By applying an inverse Fourier transform the phase can be extracted:

$$\frac{1}{\sqrt{2^n}} \sum_i \sum_x e^{-2\pi i E_i x} c_i |x\rangle |E_i\rangle \xrightarrow{QFT^{-1}} \sum_i c_i |\text{bin}(E_i)\rangle |E_i\rangle \quad (5)$$

- Therefore, by measuring the ancilla bits in the Z basis we will observe  $E_i$  to  $n$  bits with probability  $|c_i|^2$ . As  $E_i$  is likely not exact to  $n$  bits there will be a potential error introduced by the Quantum Fourier Transform, so to be accurate to  $n$  bits a few more ancilla qubits will be needed [6]. So, to find the ground energy state it needs to be in the expansion of  $|u\rangle$  and the larger the amplitude the less times QPE needs to be repeated

## 2.2 *Simulating dynamics - see Nielsen Cheung*

### 3 Jordan-Wigner Transformation

### 4 Bravyi-Kiteav Map

### 5 Derby-Klassen Map

### 6 Fermionic Enumeration

### 7 Relative performance

## 8 Introduction

The journal of *Quantum Information and Computation*, for both on-line and in-print editions, will be produced by using the latex files of manuscripts provided by the authors. It is therefore essential that the manuscript be in its final form, and in the format designed for the journal because there will be no further editing. The authors are strongly encouraged to use Rinton latex template to prepare their manuscript. Or, the authors should please follow the instructions given here if they prefer to use other software. In the latter case, the authors ought to provide a postscript file of their paper for publication.

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Major headings should be typeset in boldface with the first letter of important words capitalized.

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Sub-headings should be typeset in boldface italic and capitalize the first letter of the first word only. Section number to be in boldface roman.

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Sections, sub-sections and sub-subsections are numbered in Arabic. Use double spacing before all section headings, and single spacing after section headings. Flush left all paragraphs that follow after section headings.

### 10.3 *Lists of items*

Lists may be laid out with each item marked by a dot:

- item one,
- item two.

Items may also be numbered in lowercase roman numerals:

- (i) item one
- (ii) item two
- (a) Lists within lists can be numbered with lowercase roman letters,

(b) second item.

## 11 Equations

Displayed equations should be numbered consecutively in each section, with the number set flush right and enclosed in parentheses.

$$\mu(n, t) = \frac{\sum_{i=1}^{\infty} 1(d_i < t, N(d_i) = n)}{\int_{\sigma=0}^t 1(N(\sigma) = n) d\sigma}. \quad (6)$$

Equations should be referred to in abbreviated form, e.g. “Eq. (6)” or “(2)”. In multiple-line equations, the number should be given on the last line.

Displayed equations are to be centered on the page width. Standard English letters like  $x$  are to appear as  $x$  (italicized) in the text if they are used as mathematical symbols. Punctuation marks are used at the end of equations as if they appeared directly in the text.

**Theorem 1:** Theorems, lemmas, etc. are to be numbered consecutively in the paper. Use double spacing before and after theorems, lemmas, etc.

**Proof:** Proofs should end with  $\square$ .

## 12 Illustrations and Photographs

Figures are to be inserted in the text nearest their first reference. The postscript files of figures can be imported by using the commends used in the examples here.




fig1-eps-converted-to.pdf

Fig. 2. figure caption goes here.

Figures are to be sequentially numbered in Arabic numerals. The caption must be placed below the figure. Typeset in 8 pt Times Roman with baselineskip of 10 pt. Use double spacing between a caption and the text that follows immediately.

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### 13 Tables

Tables should be inserted in the text as close to the point of reference as possible. Some space should be left above and below the table.

Tables should be numbered sequentially in the text in Arabic numerals. Captions are to be centralized above the tables. Typeset tables and captions in 8 pt Times Roman with baselineskip of 10 pt.

Table 1. Number of tests for WFF triple NA = 5, or NA = 8.

NP					
		3	4	8	10
NC	3	1200	2000	2500	3000
	5	2000	2200	2700	3400
	8	2500	2700	16000	22000
	10	3000	3400	22000	28000

If tables need to extend over to a second page, the continuation of the table should be preceded by a caption, e.g. “(Table 2. Continued).”

### 14 References Cross-citation

References cross-cited in the text are to be numbered consecutively in Arabic numerals, in the order of first appearance. They are to be typed in brackets such as [7] and [8, 9, 10].

### 15 Sections Cross-citation

Sections and subsections can be cross-cited in the text by using the latex command shown here. In Section 15, we discuss ....

### 16 Footnotes

Footnotes should be numbered sequentially in superscript lowercase Roman letters.<sup>a</sup>

### Acknowledgements

We would thank ...

### References

References are to be listed in the order cited in the text. For each cited work, include all the authors' names, year of the work, title, place where the work appears. Use the style shown

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<sup>a</sup>Footnotes should be typeset in 8 pt Times Roman at the bottom of the page.

in the following examples. For journal names, use the standard abbreviations. Typeset references in 9 pt Times Roman.

1. Feynman, R.P.. *Simulating physics with computers*. International Journal of Theoretical Physics 1982;21(6-7):467–488. doi:10.1007/bf02650179.
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10. A.W. Marshall and I. Olkin (1979), *Inequalities: theory of majorization and its applications*, Academic Press (New York).

## Appendix A

Appendices should be used only when absolutely necessary. They should come after the References. If there is more than one appendix, number them alphabetically. Number displayed equations occurring in the Appendix in this way, e.g. (A.1), (A.2), etc.

$$\langle \hat{O} \rangle = \int \psi^*(x) O(x) \psi(x) d^3x . \quad (\text{A.1})$$