Code Generator
for Quantum Simulated Annealing

Robert R. Tucci
P.O. Box 226
Bedford, MA 01730
tucci@ar-tiste.com

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Abstract
This paper introduces QuSAnn v1.2 and Multiplexor Expander v1.2, two Java applications available for free. (Source code included in the distribution.) QuSAnn is a “code generator” for quantum simulated annealing: after the user inputs some parameters, it outputs a quantum circuit for performing simulated annealing on a quantum computer. The quantum circuit implements the algorithm of Wocjan et al. (arXiv:0804.4259), which improves on the original algorithm of Somma et al. (arXiv:0712.1008). The quantum circuit generated by QuSAnn includes some quantum multiplexors. The application Multiplexor Expander allows the user to replace each of those multiplexors by a sequence of more elementary gates such as multiply controlled NOTs and qubit rotations.

1 Introduction
For an explanation of the mathematical notation used in this paper, see some of my previous papers; for instance, Ref.[1] Section 2.

We say a unitary operator acting an array of qubits has been compiled if it has been expressed as a SEO (Sequence of Elementary Operations, like CNOTs and
single-qubit operations). SEO’s are often represented as quantum circuits.

There exist software, “general quantum compilers” (like Qubiter[2]), for compiling arbitrary unitary operators (operators that have no a priori known structure). There also exists software, “special purpose quantum compilers” (like each of the 7 applications in QuanSuite[3, 4, 5]), for compiling unitary operators that have a very definite, special structure which is known a priori.

This paper introduces QuSAnn v1.2 and Multiplexor Expander v1.2, two Java applications available for free. (Source code included in the distribution.) QuSAnn is a “code generator” for quantum simulated annealing: after the user inputs some parameters, it outputs a quantum circuit for performing simulated annealing on a quantum computer. QuSAnn is not really a quantum compiler (neither general nor special) because, although it generates a quantum circuit like the quantum compilers do, it doesn’t start with an explicitly stated unitary matrix as input. Multiplexor Expander is not a quantum compiler either for the same reason. Multiplexor Expander can be more aptly described as a “code translator”: it takes a SEO and replaces it by a different but equivalent SEO.

In Ref.[6], Somma et al. proposed an algorithm for quantum simulated annealing that requires, for any $\epsilon > 0$, order $1/\sqrt{\delta}$ elementary operations to find, with probability greater than $1 - \epsilon$, the minimum of a function. Here $\delta$ is the distance between the two largest eigenvalue magnitudes of the transition probability matrix for the Metropolis Markov chain. The algorithm of Somma et al. outperforms the classical simulated annealing algorithm, which requires order $1/\delta$ elementary operations to do the same thing.

Subsequently, Wocjan et al. in Ref.[7] improved on the algorithm of Somma et al. (See also Refs.[8, 9], where Wocjan et al. discuss related issues).

Both the Somma et al. and the Wocjan et al. algorithms use Szegedy quantum walk operators[10] and phase estimation. But the Wocjan et al. algorithm uses a Grover fixed point search[11] instead of the quantum Zeno effect.

The quantum circuit generated by QuSAnn implements the algorithm of Wocjan et al. given in Ref.[7]. The circuit includes some quantum multiplexors. (See Ref.[1] for a review of quantum multiplexors.) The application Multiplexor Expander allows the user to replace each of those multiplexors by a sequence of more elementary gates such as multiply controlled NOTs and qubit rotations. Multiplexor Expander gives the user the option of expanding the multiplexors in two different ways: either as an Exact SEO (see Refs. [2, 1]), or an Oracular Approximation (see Ref. [12]).

A nice feature of the source code for QuSAnn, Multiplexor Expander and all the applets in QuanSuite, is that they all share a common Java class library (named QLib).

2 QuSAnn

The QuSAnn applet makes the following 3 assumptions:
1. For its *annealing schedule* (see Appendix A for definition) $\beta_0, \beta_1, \beta_2, \ldots, \beta_t$, it assumes $\beta_0 = 0$ and $\beta_{j+1} - \beta_j = \Delta \beta > 0$ for all $j = 0, 1, \ldots, t_f - 1$.

2. For its *energy function* (see Appendix A for definition), it assumes $E(x) = (x - \frac{N_S}{2})^2$, where the state space (i.e., the set of $x$ values) of the minimization problem is \{0, 1, 2, \ldots, N_S - 1\}.

3. For its *neighborhood function* (see Appendix A for definition), it assumes $\text{neig}(x, y) = 1$ if $|x - y| \leq 1$ and $\text{neig}(x, y) = 0$ otherwise.

These 3 assumptions were made in order to make the applet simple. They can be easily changed (i.e, one can use a more complicated annealing schedule, energy function and neighborhood function) by making trivial alterations to the source code of QuSAnn.

### 2.1 The Control Panel

Fig[1] shows the **Control Panel** for QuSAnn. This is the main and only window of the application. This window is open if and only if the application is running.
The Control Panel allows you to enter the following inputs:

File Prefix: Prefix to the 3 output files that are written when you press the Write Files button. For example, if you insert test in this text field, the following 3 files will be written:

- test qsann log.txt
- test qsann eng.txt
- test qsann pic.txt

Some examples of these output files are given in Section 2.2 below.

Number of State Bits: The parameter $N_B = 1, 2, 3 \ldots$ defined in Appendix A. The state space of the minimization problem is \{0, 1, 2, \ldots, 2^{N_B} - 1\}. The transition
probability matrix $M$ of the Metropolis Markov chain is a $2^{N_B}$ dimensional matrix, and the Szegedy quantum walk operator $W(M)$ is a $2^{2N_B}$ dimensional matrix.

**Number of Probe Bits (for each PE step):** The parameter $a = 1, 2, 3, \ldots$ defined in Appendix D. See Fig.18.

**Number of Phase Estimation (PE) Steps:** The parameter $c = 1, 2, 3, \ldots$ defined in Appendix D. See Fig.18.

**Grover Depth:** The parameter $d_f = 1, 2, 3, \ldots$ defined in Appendix D. $d_f$ is the final level of recursion to which one wishes to carry out the fixed point Grover search.

**Upper Bound on Number of Neighbors:** The parameter $upBdNeig \in \mathbb{R} > 0$ defined in Appendix A.

**Number of Betas:** The parameter $t_f + 1 = 2, 3, \ldots$ defined above to be the number of betas in the annealing schedule.

**Delta Beta Per Unit Time:** The parameter $\Delta \beta \in \mathbb{R} > 0$ defined above to be the difference between adjacent betas of the annealing schedule.

The Control Panel displays the following outputs:

**Number of Qubits:** The total number of qubits used by the circuit, equal to $2N_B + ac$ in the notation of Appendix D.

**Number of Elementary Operations:** The number of elementary operations in the output quantum circuit. If there are no LOOPS, this is the number of lines in the English File (see Sec. 2.2.2), which equals the number of lines in the Picture File (see Sec. 2.2.3). For a LOOP (which is not nested inside a larger LOOP), the “LOOP k REPS: N” and “NEXT k” lines are not counted, whereas the lines between “LOOP k REPS: N” and “NEXT k” are counted $N$ times. Multiplexors expressed as a single line are counted as a single elementary operation (unless, of course, they are inside a LOOP, in which case they are used repeatedly).

**Message:** A message appears in this text field if you press Write Files with a bad input. The message tries to explain the mistake in the input.

### 2.2 Output Files

Figs. 2, 3 and 4 were all generated in a single run of QuSAnn (by pressing the Write Files button just once). They are examples of what we call the Log File, English File, and Picture File, respectively, of QuSAnn. Next we explain the contents of each of these output files.
2.2.1 Log File

Fig. 2 is an example of a Log File. The Log File records all the information found in the Control Panel.

2.2.2 English File

Fig. 3 is an example of an English File. The English File completely specifies the output SEO. It does so “in English”, thus its name. Each line represents one elementary operation, and time increases as we move downwards.

In general, an English File obeys the following rules:

- Time grows as we move down the file.
- Each row corresponds to one elementary operation. Each row starts with 4 letters that indicate the type of elementary operation.
- For a one-bit operation acting on a “target bit” \( \alpha \), the target bit \( \alpha \) is given after the word AT.
- If the one-bit operation is controlled, then the controls are indicated after the word IF. T and F stand for true and false, respectively. \( \alpha T \) stands for a control \( n(\alpha) \) at bit \( \alpha \). \( \alpha F \) stands for a control \( \overline{n}(\alpha) \) at bit \( \alpha \).
- “LOOP \( k \) REPS: N” and “NEXT \( k \)” mark the beginning and end of \( N \) iterations. \( k \) labels the loop. \( k \) also equals the line-count number (first line is 0) of the line “LOOP \( k \) REPS: N” in the English file.
- **SWAP** $\alpha \beta$ stands for the swap(exchange) operator $E(\alpha, \beta)$ that swaps bits $\alpha$ and $\beta$.

- **PHAS** $\theta^{\text{deg}}$ stands for a phase factor $e^{i\theta^{\text{deg}} \frac{\pi}{180}}$.

- **POPH** $\theta^{\text{deg}}$ stands for the one-bit gate $e^{iP_0\theta^{\text{deg}} \frac{\pi}{180}}$. **P1PH** $\theta^{\text{deg}}$ stands for the one-bit gate $e^{iP_1\theta^{\text{deg}} \frac{\pi}{180}}$. Target bit follows the word AT.

- **SIGX, SIGY, SIGZ, HAD2** stand for the Pauli matrices $\sigma_X, \sigma_Y, \sigma_Z$ and the one-bit Hadamard matrix $H$, respectively. Target bit follows the word AT.

- **ROTX, ROTY, ROTZ, ROTN** stand for one-bit rotations with rotation axes in the directions: $x$, $y$, $z$, and an arbitrary direction $n$, respectively. Rotation angles (in degrees) follow the words ROTX, ROTY, ROTZ, ROTN. Target bit follows the word AT.

- **MP_Y** stands for a multiplexor which performs a one-bit rotation of a target bit about the $y$ axis. Target bit follows the word AT. Rotation angles (in degrees) follow the word BY. Multiplexor controls are specified by $\alpha(k)$, where integer $\alpha$ is the bit position and integer $k$ is the control's name.

Figure 3: English File generated by QuSann in the same run as the Log File of Fig.2. Bottom of file is not visible. Right hand side of file is not visible.
Figure 4: Picture File generated by QuSAnn in the same run as the Log File of Fig[2].
Bottom of file is not visible.

used in Ref.[1] into the English File language[1]

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1 This same table appeared before in Ref.[3] except that we have added a new row of boxes at the end of the table for multiplexors expressed as a single line in the English and Picture files.
Mathematical language | English File language
--- | ---
Loop named 5 with 2 repetitions | LOOP 5 REPS: 2
Next iteration of loop named 5 | NEXT 5
$E(1, 0)^{n(2)}$ | SWAP 1 0 IF 3F 2T
$e^{i42.7\frac{\pi}{180}}n(2)$ | PHAS 42.7 IF 3F 2T
$e^{i42.7\frac{\pi}{180}}n(2)$ | P0PH 42.7 AT 3 IF 2T
$e^{i42.7\frac{\pi}{180}}n(2)$ | P1PH 42.7 AT 3 IF 2T
$\sigma_X(1)n(2)$ | SIGX AT 1 IF 3F 2T
$\sigma_Y(1)n(2)$ | SIGY AT 1 IF 3F 2T
$\sigma_Z(1)n(2)$ | SIGZ AT 1 IF 3F 2T
$H(1)n(2)$ | HAD2 AT 1 IF 3F 2T
$(e^{i\frac{\pi}{180}23.7}\sigma_X(1))n(2)$ | ROTX 23.7 AT 1 IF 3F 2T
$(e^{i\frac{\pi}{180}23.7}\sigma_Y(1))n(2)$ | ROTY 23.7 AT 1 IF 3F 2T
$(e^{i\frac{\pi}{180}23.7}\sigma_Z(1))n(2)$ | ROTZ 23.7 AT 1 IF 3F 2T
$(e^{i\frac{\pi}{180}[30\sigma_X(1)+40\sigma_Y(1)+11\sigma_Z(1)]}n(2)$ | ROTN 30.0 40.0 11.0 AT 1 IF 3F 2T
$[e^{i\sum_{b_1,b_0}\theta_{b_1b_0}\sigma_Y(3)P_{b_1b_0}(2,1)}]n(0)$ | MP_Y AT 3 IF 2(1 1(0 0T BY 30.0 10.5 11.0 83.1
where $\left\{
\begin{align*}
\theta_{00} &= 30.0(\frac{\pi}{180}) \\
\theta_{01} &= 10.5(\frac{\pi}{180}) \\
\theta_{10} &= 11.0(\frac{\pi}{180}) \\
\theta_{11} &= 83.1(\frac{\pi}{180})
\end{align*}\right.$

2.2.3 ASCII Picture File

Fig 4 is an example of a Picture File. The Picture File partially specifies the output SEO. It gives an ASCII picture of the quantum circuit. Each line represents one elementary operation, and time increases as we move downwards. There is a one-to-one onto correspondence between the rows of the English and Picture Files.

In general, a Picture File obeys the following rules:

- Time grows as we move down the file.
- Each row corresponds to one elementary operation. Columns 1, 5, 9, 13, ... represent qubits (or, qubit positions). We define the rightmost qubit as 0. The
qubit immediately to the left of the rightmost qubit is 1, etc. For a one-bit operator acting on a “target bit” \( \alpha \), one places a symbol of the operator at bit position \( \alpha \).

- \( | \) represents a “qubit wordline” connecting the same qubit at two consecutive times.
- \( - \) represents a wire connecting different qubits at the same time.
- \( + \) represents both \( | \) and \( - \).

- If the one-bit operation is controlled, then the controls are indicated as follows. 
  \( @ \) at bit position \( \alpha \) stands for a control \( n(\alpha) \).  \( 0 \) at bit position \( \alpha \) stands for a control \( \overline{n(\alpha)} \).

- “\( \text{LOOP } k \ \text{REPS}:N \)” and “\( \text{NEXT } k \)” mark the beginning and end of \( N \) iterations. \( k \) labels the loop. \( k \) also equals the line-count number (first line is 0) of the line “\( \text{LOOP } k \ \text{REPS}:N \)” in the Picture File.

- The swap(exchange) operator \( E(\alpha, \beta) \) is represented by putting arrow heads < and > at bit positions \( \alpha \) and \( \beta \).

- A phase factor \( e^{i\theta} \) for \( \theta \in \mathbb{R} \) is represented by placing \( \text{Ph} \) at any bit position which does not already hold a control.

- The one-bit gate \( e^{iP_0(\alpha)\theta} \) for \( \theta \in \mathbb{R} \) is represented by putting \( \text{OP} \) at bit position \( \alpha \).

- The one-bit gate \( e^{iP_1(\alpha)\theta} \) for \( \theta \in \mathbb{R} \) is represented by putting \( \oplus \text{P} \) at bit position \( \alpha \).

- One-bit operations \( \sigma_X(\alpha), \sigma_Y(\alpha), \sigma_Z(\alpha) \) and \( H(\alpha) \) are represented by placing the letters \( X,Y,Z,H \), respectively, at bit position \( \alpha \).

- One-bit rotations acting on bit \( \alpha \), in the \( x,y,z,n \) directions, are represented by placing \( Rx, Ry, Rz, R \), respectively, at bit position \( \alpha \).

- A multiplexor that rotates a bit \( \tau \) about the \( y \) axis is represented by placing \( Ry \) at bit position \( \tau \). A multiplexor control at bit position \( \alpha \) and named by the integer \( k \) is represented by placing \( (k \) at bit position \( \alpha \).

Here is a list of examples showing how to translate the mathematical notation used in Ref.[1] into the Picture File language\(^2\)

\(^2\) This same table appeared before in Ref.[3] except that we have added a new row of boxes at the end of the table for multiplexors expressed as a single line in the English and Picture files.
3 Multiplexor Expander

QuSAnn outputs a quantum circuit which includes multiplexor operations. Multiplexor Expander can read the output files of QuSAnn and write new files in which each multiplexor is replaced by a sequence of more elementary operations such as multiply controlled NOTs and single qubit rotations. Multiplexor Expander gives the user the option of expanding the multiplexors in two different ways: either as an Exact SEO (see Ref. [2, 1]), or an Oracular Approximation (see Ref. [12]).
3.1 The Control Panel

Fig 5 shows the Control Panel for Multiplexor Expander. This is the main and only window of the application. This window is open if and only if the application is running.

![Control Panel of Multiplexor Expander](image)

The Control Panel allows you to enter the following inputs:

**Prefix for Input Files:** Prefix to the 2 input files that are read when you press the Write Output Files button. For example, if you insert `testIn_qexp` in this text field, the following 2 files will be read:

- `testIn_qexp_eng.txt`
- `testIn_qexp_pic.txt`

Some examples of these input files are given in Section 3.2 below. These 2 files are usually English File and Picture File outputted by QuSAnn. If they aren’t, they must be formatted in the same way as the 2 files outputted by QuSAnn or else Multiplexor Expander will fail.

**Prefix for Output Files:** Prefix to the 3 output files that are written when you press the Write Output Files button. For example, if you insert `testOut_qexp` in this text field, the following 3 files will be written:
Some examples of these output files are given in Section 3.3 below.

**Compilation Mode:** The compilation mode, either as Exact SEO (see Ref. [2, 1]), or Oracular Approximation (see Ref. [12]).

**Bit Precision:** The number of significant fractional bits in the oracular approximation (see Ref. [12]). This parameter is ignored if the compilation mode is Exact SEO.

The Control Panel displays the following outputs:

**Number of Elementary Operations:** Same as in QuSAnn Control Panel.

**Message:** Same as in QuSAnn Control Panel.

### 3.2 Input Files

Figs. 6 and 7 are examples of the 2 input files for Multiplexor Expander, what we call the **Input English File** and **Input Picture File**, respectively, of Multiplexor Expander. These examples are not really output files of QuSAnn, but they are formatted in the same way as English and Picture files of QuSAnn.

![Figure 6: Input English File for Multiplexor Expander.](testIn_qexp_eng.txt)

![Figure 7: Input Picture File for Multiplexor Expander.](testIn_qexp_pic.txt)

Figure 6: Input English File for Multiplexor Expander. Right hand side of file is not visible.

Figure 7: Input Picture File for Multiplexor Expander.
3.3 Output Files

Figs. 8, 9 and 10 were all generated in a single run of Multiplexor Expander (by pressing the Write Output Files button just once), with

- the input files of Figs. 6 and 7, and
- the compilation mode set to **Exact SEO**.

Figs. 8, 9 and 10 are examples of what we call the **Output Log File, Output English File, and Output Picture File**, respectively, of Multiplexor Expander. The notation of these files is the same as that for the Log, English and Picture files for QuSAnn (see Section 2.2).

Figs. 11, 12 and 13 are similar to Figs. 8, 9 and 10 above, except that they were all generated in a single run of Multiplexor Expander, with

- the input files of Figs. 6 and 7, and
- the compilation mode set to **Oracular Approximation**.

![Figure 8: Output Log File generated by Multiplexor Expander with Exact SEO as compilation mode.](image)
Figure 9: Output English File generated by Multiplexor Expander in the same run as the Log File of Fig.

Figure 10: Output Picture File generated by Multiplexor Expander in the same run as the Log File of Fig.
Figure 11: Output Log File generated by Multiplexor Expander with Oracular Approximation as compilation mode.

Figure 12: Output English File generated by Multiplexor Expander in the same run as the Log File of Fig.11.

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A Appendix: Classical Simulated Annealing

The goal of simulated annealing, both classical and quantum, is to find the minimum of a (bounded below) function (i.e. to solve a minimization problem). The function $E : S_x \rightarrow \mathbb{R}^{\geq 0}$ to be minimized will be called the energy function (assumed non-negative without loss of generality). It’s domain $S_x$ will be called the state space. We will assume that $S_x = \{0, 1, 2, \ldots, N_S - 1\}$, were $N_S = 2^{N_B}$ is the number of states and $N_B$ is the number of bits. Besides the state space and energy function, it is also convenient to introduce a neighborhood function $\text{neig} : S_x \times S_x \rightarrow \text{Bool}$, defined by $\text{neig}(x, y) = \theta(x \text{ and } y \text{ are neighbors})$.

To solve this minimization problem, classical simulated annealing uses a Markov chain.

A Markov chain is a Bayesian network $x_0 \rightarrow x_1 \rightarrow \cdots \rightarrow x_t$, wherein all random variables $x_j \in S_{x_j}$ have the same range of values: $S_{x_j} = S_x$ for all $j$, and every node except the first one has the same transition probability matrix: $P_{x_{j+1}|x_j}(y|x) = M(y|x)$ for $j = 0, 1, \ldots, t_f - 1$ and $x, y \in S_x$. A stationary state $\pi()$ of the Markov chain with transition probability matrix $M$ is a probability distribution on $S_x$ which is also an eigenstate of $M$ with unit eigenvalue,

$$\sum_{x \in S_x} M(y|x)\pi(x) = \pi(y) \quad (1)$$

for all $y \in S_x$. We say that a probability distribution $\pi(x)$ is a detailed balance of
for all $x, y \in S_x$. Clearly, if $\pi()$ is a detailed balance of $M$, it is also a stationary state of it.

Classical simulated annealing uses a special Markov chain due to Metropolis. The Metropolis transition probability matrix $M_\beta$ for a given minimization problem and inverse temperature $\beta > 0$, is defined as follows:

$$M_\beta(y|x) = \begin{cases} \theta(x \neq y) \frac{\text{neig}(x,y)}{\text{upBdNeig}} \min\{1, e^{-\beta[E(y)-E(x)]}\} \\ +\theta(x = y) \left(1 - \sum_{z,z \neq x} M_\beta(z|x)\right) \end{cases},$$

where upBdNeig is some real number greater or equal to $\max_y \sum_x \text{neig}(x, y)$. Thus, upBdNeig is an upper bound on the number of neighbors. Fig. 14 tries to explain the logic behind Eq. (3). A “system” prefers going downhill to going uphill, but is willing to visit a neighbor living uphill occasionally.

One can show that the following probability distribution (called a normalized Boltzmann factor) is a detailed balance and therefore a stationary distribution of $M_\beta$.

$$\pi_\beta(x) = \frac{e^{-\beta E(x)}}{Z_\beta}.$$  

$Z_\beta$ is called the partition function. It is defined so as to make $\pi()$ a probability distribution:

$$Z_\beta = \sum_x e^{-\beta E(x)}.$$

In classical simulated annealing, we consider a product $M_{\beta_f} \ldots M_{\beta_1} M_{\beta_0}$ of transition probability matrices. The monotonically increasing (or at least non-decreasing) sequence of non-negative real numbers $\beta_0, \beta_1, \ldots, \beta_{tf}$ is called the annealing schedule.
Appendix: Q-Embedding of Probability Matrix

In this Appendix, we will review the concept of q-embedding of a probability matrix, as used in Ref. [13] and later in Ref. [14].

Given a conditional probability \( P(y|x) \) where \( x \in S_x \) and \( y \in S_y \), we will call a probability matrix the matrix \( P \) with entries \( P(y|x) \) with rows labeled by the \( y \) and columns by the \( x \). Any unitary matrix \( U \) with matrix elements \( \langle y|\langle \tilde{x}|U|\tilde{y}\rangle|x \rangle = A(y, \tilde{x}|\tilde{y}, x) \), where \( x, \tilde{x} \in S_x \) and \( y, \tilde{y} \in S_y \), that satisfies

\[
\sum_{\tilde{x}} |A(y, \tilde{x}|\tilde{y} = 0, x)|^2 = P(y|x),
\]

for all \( x, y \), will be called a q-embedding (quantum-embedding) of the probability matrix \( P \). \( A() \) acts like a probability amplitude. The index \( \tilde{y} \) that we set to a fixed value (call it zero) is called a source and the index \( \tilde{x} \) that we sum over is called a sink. This nomenclature is similar to the one used by Fredkin and Toffoli when they showed how any boolean function \( f: \text{Bool}^m \rightarrow \text{Bool}^n \) can be embedded in a reversible function. See Ref. [13] for more details and references. Note that Eq. (6) is satisfied if we set

\[
A(y, \tilde{x}|\tilde{y} = 0, x) = \delta_{\tilde{x}} \sqrt{P(y|x)}.
\]

A q-embedding of a probability matrix is of course not unique. Next we will give one possible q-embedding for any square probability matrix acting on \( N_B \) bits. The q-embedding that we will give is very convenient because it is expressed succinctly as a product of quantum multiplexors. (See Ref. [1] for a review of quantum multiplexors).

We begin by pointing out some trivial algebraic results that will be used below. Note that for any \( \theta \in \mathbb{R} \),

\[
e^{-i\sigma_y \theta} = \begin{bmatrix} C_\theta & -S_\theta \\ S_\theta & C_\theta \end{bmatrix}.
\]

\( C_\theta, S_\theta \) are shorthand for \( \cos \theta \) and \( \sin \theta \), respectively. Thus, if \( b \in \text{Bool} \), we get from the first column of this matrix that:

\[
\langle b|e^{-i\sigma_y \theta}|0 \rangle = C_\theta^b S_\theta^b = \begin{cases} C_\theta & \text{if } b = 0 \\ S_\theta & \text{if } b = 1 \end{cases}.
\]

We are using the notation of Ref. [1] for \( \overline{b} \) where \( b \in \text{Bool} \), namely \( \overline{0} = 1 \) and \( \overline{1} = 0 \). A compact expression for the entries of both columns can be obtained as follows. For \( a, b \in \text{Bool} \),

\[
\langle b|e^{-i\sigma_y \theta}|a \rangle = \langle b|e^{-i\sigma_y \theta} \sigma_x^a|0 \rangle = \langle b \oplus a|e^{-i(-1)^a \sigma_y \theta}|0 \rangle.
\]
The last matrix element in Eq. (10) is given by Eq. (9).

Let \( q \in \mathbb{R}^{N_S \times N_S} \) be the probability matrix for which we desire a q-embedding.

First consider \( N_B = 1 \). We want the following constraint to be satisfied:

\[
A(b_1, b_0 | a_1 = 0, a_0) = \delta_{b_0}^{a_0} \sqrt{q(b_1 | a_0)},
\]

where \( b_1, b_0, a_1, a_0 \in \text{Bool} \). Define a unitary matrix \( \tilde{U} \) by

\[
\tilde{U} = e^{-i \sum a_0 \sigma_Y(1) \theta_{|a_00}, 0)},
\]

where the angles \( \theta_{|a_00} \) are defined by

\[
C_{\theta_{|a_00}}^{2b_1} S_{\theta_{|a_00}}^{b_1} = q_{b_1 | a_0}.
\]

Using \( P_b | b' \rangle = \delta_b^b | b \rangle \) for \( b, b' \in \text{Bool} \), and Eq. (9) it follows that

\[
\langle b_0 | \tilde{U} | a_0 \rangle = \delta_{b_0}^{a_0} \langle b_1 | e^{-i \sigma_Y(1) \theta_{|a_00}, 0} | 0 \rangle
\]

\[
= \delta_{b_0}^{a_0} \delta_{b_1}^{2b_1} S_{\theta_{|a_00}}^{b_1}
\]

\[
= \delta_{b_0}^{a_0} \sqrt{q_{b_1 | a_0}}.
\]

Hence \( \tilde{U} \) is a q-embedding of \( q \).

Now consider \( N_B = 2 \). We want

\[
A(b_3, b_2, b_1, b_0 | a_3 = 0, a_2 = 0, a_1, a_0) = \delta_{b_3}^{a_3} \delta_{b_0}^{a_0} \sqrt{q(b_3, b_2 | a_1, a_0)},
\]

where all \( a_j \) and \( b_j \) are in \( \text{Bool} \). Define a unitary matrix \( \tilde{U} \) by

\[
\tilde{U} = e^{-i \sum b_2, a_1, a_0 \sigma_Y(3) \theta_{b_2|a_1a_0}, P_{b_2a_1a_0}(2, 1, 0) e^{-i \sum a_1, a_0 \sigma_Y(2) \theta_{|a_1a_0}, P_{a_1a_0}(1, 0)}},
\]

where the angles \( \theta_{b_2|a_1a_0} \) and \( \theta_{|a_1a_0} \) are defined by

\[
C_{\theta_{b_2|a_1a_0}}^{2b_3} S_{\theta_{|a_1a_0}}^{b_3} = q_{b_3b_2|a_1a_0} / q_{b_2|a_1a_0},
\]

and

20
\[ C_{\theta_{a_1a_0}}^{b_2} S_{\theta_{a_1a_0}}^{b_2} = q.b_2|a_1a_0 \]  \hspace{1cm} (18)

(We are using the notation of Ref.[1] where a dot at the position of an index means that the index has been summed over; e.g., \( q.b = \sum_a q_{ab} \)). It follows that

\[
\langle b_0 | \cdots a_0 \rangle = \delta_{b_1}^{a_1} \delta_{b_0}^{a_0} \langle b_3 | e^{-i\sigma_Y(3)} | b_{a_1a_0} \rangle \langle 0 | b_2 | e^{-i\sigma_Y(2)} | b_{a_1a_0} \rangle \hspace{1cm} (19a)
\]

\[
\langle b_1 | \cdots a_1 \rangle = \delta_{b_1}^{a_1} \delta_{b_0}^{a_0} C_{b_2|a_1a_0}^{b_3} S_{b_2|a_1a_0}^{b_3} \hspace{1cm} (19b)
\]

\[
\langle b_2 | \cdots 0 \rangle = \delta_{b_1}^{a_1} \delta_{b_0}^{a_0} \sqrt{q_{b_3b_2|a_1a_0}} \hspace{1cm} (19c)
\]

Thus, as in the \( N_B = 1 \) case, \( \bar{U} \) is a \( q \)-embedding of \( q \).

It’s clear how to generalize this construction so as to get a \( q \)-embedding of a probability matrix \( q \in \mathbb{R}^{N_S \times N_S} \) for any positive integer \( N_B \).

### C Appendix: Szegedy Quantum Walk Operator \( W \)

In this appendix, we will review the definition and some useful properties of the Szegedy quantum walk operator \( W \) (first defined by Szegedy in Ref.[10], first used for simulated annealing by Somma et al. in Ref.[6], first implemented in terms of multiplexors here).

#### C.1 Symmetric Matrix \( M_{\text{sym}} \)

For any Markov chain with transition probability \( M \), define matrix \( \Lambda \) (the entry-wise square root of \( M \)) by

\[
\Lambda(y|x) = \sqrt{M(y|x)} , \hspace{1cm} (20)
\]

and the matrix \( M_{\text{sym}} \) (a symmetric version of \( M \)) by

\[
M_{\text{sym}}(y|x) = \Lambda(x|y)\Lambda(y|x) , \hspace{1cm} (21)
\]

for all \( x, y \in S_2 \). (Note that unlike \( M(y|x) \), \( M_{\text{sym}}(y|x) \) is not a probability function in \( y \), its first argument.)

Define the quantum states

\[
|\!(\pi)^{\eta} \rangle = \sum_x [\pi(x)]^{\eta}|x\rangle \hspace{1cm} (22)
\]
for $\eta = \frac{1}{2}, 1$. (Note that only the $\eta = \frac{1}{2}$ state is normalized in the sense of quantum mechanics.)

**Claim 1**

$$M|\pi\rangle = |\pi\rangle,$$  \hspace{1cm} (23)

and

$$M_{\text{sym}}|\sqrt{\pi}\rangle = |\sqrt{\pi}\rangle.$$  \hspace{1cm} (24)

Also, $M$ and $M_{\text{sym}}$ have the same eigenvalues.

**proof:**

Taking the square root of both sides of the detailed balance statement Eq.(2), we get

$$\Lambda(y|x)\sqrt{\pi(x)} = \Lambda(x|y)\sqrt{\pi(y)}.$$  \hspace{1cm} (25)

Therefore,

$$M_{\text{sym}}(y|x) = \Lambda(x|y)\frac{1}{\sqrt{\pi(x)}}\Lambda(x|y)\sqrt{\pi(y)} = \frac{1}{\sqrt{\pi(x)}}M(x|y)\sqrt{\pi(y)}.$$  \hspace{1cm} (26a)

Hence,

$$\sum_x M(y|x)\pi(x) = \sum_x M(x|y)\pi(y) = \pi(y),$$  \hspace{1cm} (27)

and

$$\sum_x M_{\text{sym}}(y|x)\sqrt{\pi(x)} = \sum_x \frac{1}{\sqrt{\pi(x)}}M(x|y)\sqrt{\pi(y)}\sqrt{\pi(x)} = \sqrt{\pi(y)}.$$  \hspace{1cm} (28)

Order the elements of the finite set $S_x$ in some preferred way. Use this preferred order to represent $M$ and $M_{\text{sym}}$ as matrices. Define a diagonal matrix $D$ whose diagonal entries are the numbers $\pi(x)$ for each $x \in S_x$, with the $x$ ordered in the preferred order:

$$D = \text{diag}[\pi(x)]_x.$$  \hspace{1cm} (29)

Since

$$M_{\text{sym}} = D^{-\frac{1}{2}}MD^\frac{1}{2},$$  \hspace{1cm} (30)

it follows that
\[ \det(M - \lambda) = \det(M_{sym} - \lambda) \] (31)

for any \( \lambda \in \mathbb{R} \).

**QED**

Let the eigenvalues of \( M_{sym} \) (and also of \( M \)) be \( m_0, m_1, \ldots, m_{N_S - 1} \in \mathbb{R} \) with \( m_0 = 1 \geq |m_1| \geq |m_2| \ldots \geq |m_{N_S - 1}| \). Define \( |m_j\rangle \) to be the corresponding eigenvectors of \( M_{sym} \) (but not necessarily of \( M \)). Thus

\[ M_{sym} |m_j\rangle = m_j |m_j\rangle, \] (32)

for \( j = 0, 1, \ldots, N_S - 1 \). In particular, \( |m_0\rangle = |\sqrt{\pi}\rangle \).

For each \( j \), define \( \varphi_j \in [0, \frac{\pi}{2}] \) and \( \eta_j \in \{0, \pi\} \) so that \( m_j = e^{i\eta_j} \cos \varphi_j \). (Thus, \( \cos \varphi_j \geq 0 \) and \( e^{i\eta_j} = \pm 1 \)). Note that \( m_0 = 1 \) so \( \varphi_0 = 0 \). The \( M \) eigenvalue gap \( \delta \) is defined as \( \delta = 1 - |m_1| \). \( \delta \approx \frac{\varphi_1^2}{2} \) when \( \varphi_1 \) is small.

### C.2 Q-Embeddings \( \tilde{U} \) and \( \hat{U} \)

Next we will consider two “dual” disjoint sets of distinct qubits with \( N_B \) qubits in each set. Let these two set be labeled \( \vec{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_{N_B}) \) and \( \vec{\beta} = (\beta_1, \beta_2, \ldots, \beta_{N_B}) \). Any operator \( \Omega \) acting on the tensor product of a state \( |x\rangle_{\vec{\alpha}} \) and a state \( |y\rangle_{\vec{\beta}} \) where \( x, y \in \text{Bool}^{N_B} \), can be represented, depending on taste, either in quantum circuit notation or Dirac notation, by

\[ \begin{array}{c}
\hline
\Omega & |x\rangle_{\vec{\alpha}} \\
\hline
|y\rangle_{\vec{\beta}} & \end{array} = \begin{array}{c}
\Omega |y\rangle_{\vec{\beta}} |x\rangle_{\vec{\alpha}} \\
\end{array} . \] (33)

Let \( \uparrow \) denote the operator that swaps all bits \( \alpha_j \) and \( \beta_j \) for \( j = 1, 2, \ldots, N_B \). Let \( \tilde{U} \) be any unitary matrix satisfying for any \( x \in \text{Bool}^{N_B} \),

\[ \begin{array}{c}
\hline
\tilde{U} & |x\rangle \\
\hline
|0\rangle & (\Lambda |x\rangle) \\
\end{array} = |x\rangle \] or \( \tilde{U} |0\rangle |x\rangle = (\Lambda |x\rangle)|x\rangle . \] (34)

Let

\[ \tilde{A}(y', y|0, x) = \begin{array}{c}
\hline
\tilde{U} & |x\rangle \\
\hline
\langle y'| & |y\rangle \end{array} \begin{array}{c}
\langle y'| & |x\rangle \\
\hline
|0\rangle & \end{array} = \langle y'| |y\rangle |0\rangle |x\rangle . \] (35)

for \( x, 0, y, y' \in \text{Bool}^{N_B} \). Then, by virtue of Eq.(34),

---

3 There must be a single eigenvalue 1 and all others must have a magnitude strictly smaller than one because of the Frobenius-Perron Theorem. The eigenvalues must be real (but they can be negative) because \( M_{sym} \) is a Hermitian matrix.
Thus, $\hat{U}$ is a q-embedding of the probability matrix $M$.

If we define $\hat{U}$ by

$$\hat{U} = \uparrow \hat{\tilde{U}} \uparrow,$$  \hfill (37)

then we can immediately write the following equations, which are dual to equations we wrote previously for $\hat{U}$:

$$\hat{A}(y', y | x, 0) = \langle y | \hat{U} | 0 \rangle \langle y' \Lambda | x \rangle = \langle y' | \hat{U} | x \rangle \langle y | 0 \rangle \Lambda(x) = \delta(y', x) \Lambda(y | x) = \delta(y', x) \sqrt{M(y | x)}. \hfill (38)$$

Next define the unitary operator $U$ by

$$U = \hat{U}^\dagger \hat{\tilde{U}}. \hfill (41)$$

Clearly,

$$\uparrow \downarrow U = U^\dagger. \hfill (42)$$

Note that $U$ $\uparrow$ is Hermitian and its square equals one:

$$(U \uparrow)^\dagger = \uparrow \downarrow U = U \uparrow, \quad (U \uparrow)^2 = 1. \hfill (43)$$

Matrix $U$ has the following highly desirable property:

**Claim 2** For any $j, k \in \{0, 1, \ldots, N - 1\}$,

$$\langle 0 | \hat{U} | m_k \rangle = m_j \delta_j^k. \hfill (44)$$

**proof:**

$$\langle 0 | \hat{U} | m_k \rangle = \sum_{y, x} \langle m_j | y \rangle \langle y | \Lambda T \rangle \Lambda(x) \langle x | m_k \rangle = m_j \delta_j^k.$$  \hfill (45a)

$$\langle 0 | \hat{U} | m_k \rangle = \sum_{y, x} \langle m_j | y \rangle \Lambda T(y | x) \Lambda(y | x) \langle x | m_k \rangle = m_j \delta_j^k. \hfill (45b)$$

$$\langle 0 | \hat{U} | m_k \rangle = m_j \delta_j^k. \hfill (45c)$$
QED

C.3 Definition of $W$

Now define the projection operator $\hat{\pi}$ by (expressed below in 3 alternative but equivalent notations)

$$\hat{\pi} = \begin{bmatrix} 0 \langle \end{bmatrix} = I_2^{\otimes NB} \otimes P_0^{\otimes NB} = P_0(\vec{a}) .$$  \hspace{1cm} (46)

Define the projection operator $\check{\pi}$ dual to $\hat{\pi}$, by

$$\check{\pi} = \hat{\pi} = \begin{bmatrix} 0 \langle \end{bmatrix} .$$ \hspace{1cm} (47)

Define a reflection operator $(-1)^\hat{\pi}$ (expressed below in several equivalent notations) and its dual reflection operator $(-1)^\check{\pi}$ as follows:

$$(-1)^\hat{\pi} = 1 - 2\hat{\pi} = I_2^{\otimes NB} \otimes (-1)^{P_0^{\otimes NB}} = (-1)\prod_{j=1}^{N_B} \pi(\alpha_j) ,$$  \hspace{1cm} (48)

$$(-1)^\check{\pi} = \check{\pi} \check{\pi} .$$  \hspace{1cm} (49)

Finally (gasp!), we are ready to define the Szegedy quantum walk operator $W$ corresponding to the transition probability matrix $M$, by

$$W(M) = U(-1)^\check{\pi}U^\dagger(-1)^\hat{\pi} .$$  \hspace{1cm} (50)

C.4 Eigenvalues of $W$

To find the eigenvalues of $W$, we will use the following identities.

Claim 3

$$\hat{\pi}|m_j0\rangle = |m_j0\rangle ,$$  \hspace{1cm} (51a)

$$\hat{\pi}(U \dagger)|m_j0\rangle = m_j|m_j0\rangle ,$$  \hspace{1cm} (51b)

for all $j \in \{0, 1, \ldots, N_S - 1\}$.

proof:

From the definition of $\hat{\pi}$, we see that

$$\hat{\pi} \begin{bmatrix} 0 \\ |m_j\rangle \end{bmatrix} = \begin{bmatrix} 0 \\ |m_j\rangle \end{bmatrix} .$$  \hspace{1cm} (52)
Also,

\[ \hat{\pi}(U \uparrow) |m_j\rangle = \sum_k |m_k\rangle \langle m_k| U |m_j\rangle = m_j |m_j\rangle. \]  

(53)

QED

An immediate consequence of Claim 3 is that

\[ \langle m_j | U \uparrow | m_k \rangle = \langle m_j | \hat{\pi} U \uparrow | m_k \rangle = m_j \delta_j^k, \]  

(54)

for \( j, k \in \{0, 1, \ldots, N_S - 1\} \).

Note that since \( m_0 = 1 \), Eq. (54) implies that

\[ |m_0\rangle = U \uparrow |m_0\rangle. \]  

(55)

Another consequence of Claim 3 is that \( |m_0\rangle \) is a stationary state of \( W \).

Indeed, one has

\[ W |m_0\rangle = U (-1)^j U^\dagger (-1)^j |m_0\rangle \]

\[ = U \uparrow (1 - 2\hat{\pi}) \downarrow U^\dagger (-1)|m_0\rangle \]  

(56a)

\[ = (1 - 2m_0 U \uparrow)(-1)|m_0\rangle \]  

(56b)

\[ = (1 - 2)(-1)|m_0\rangle \]  

(56c)

\[ = |m_0\rangle. \]  

(56d)

(56e)

Let

\[ \mathcal{V}_j^{\text{busy}} = \text{span}\{|m_j\rangle, U \uparrow |m_j\rangle\} \]  

(57)

for \( j \in \{0, 1, \ldots, N_S - 1\} \). (By “span” we mean all linear combinations of these vectors with complex coefficients.)

Claim 4 \( W \mathcal{V}_j^{\text{busy}} = \mathcal{V}_j^{\text{busy}} \) for all \( j \in \{0, 1, \ldots, N_S - 1\} \). For \( j = 0 \), let

\[ |\psi_0\rangle = |m_0\rangle. \]  

(58)

\{\|\psi_0\rangle\} is an orthonormal basis for \( \mathcal{V}_0^{\text{busy}} \) and \( W |\psi_0\rangle = |\psi_0\rangle \). For \( j \neq 0 \), let

\[ |\psi_{\pm j}\rangle = \frac{\pm i}{\sqrt{2 \sin \varphi_j}} (e^{-i\varphi_j} U \uparrow |m_j0\rangle - e^{i2\varphi_j} |m_j0\rangle) \]  

(59)

\{\|\psi_j\rangle, |\psi_{-j}\rangle\} is an orthonormal basis for \( \mathcal{V}_j^{\text{busy}} \) and \( W |\psi_{\pm j}\rangle = e^{i2\varphi_j} |\psi_{\pm j}\rangle \).

proof:

Using the identities of Claim 3 one finds after some algebra that
\[ W|m_j0⟩ = (-1)|m_j0⟩ + (2m_j)U \downarrow |m_j0⟩ \]  
\[ \text{and} \]
\[ W(U \uparrow)|m_j0⟩ = (-2m_j)|m_j0⟩ + (-1 + 4m_j^2)U \downarrow |m_j0⟩ \]  
for all \( j \).

According to Eqs. (60), \( V_{bus} \) is invariant under the action of \( W \) for each \( j \). By virtue of Eq. (54), \( V_{bus} \) is 1-dim for \( j = 0 \) and 2-dim if \( j \neq 0 \). We’ve already proven that \( |m_00⟩ \) is a stationary state of \( W \).

Now consider the case \( j \neq 0 \). Both \( U(−1)^{\#}U^\dagger \) and \( (−1)^{\#} \) are reflections in the planar subspace \( V_{bus} \), and reflections are a special type of rotation about the axis normal to this plane, so their product is also a rotation about this axis. The vectors \( |m_j0⟩ \), and \( U \downarrow |m_j0⟩ \) are independent but not orthogonal. However, we can express them in terms of orthogonal vectors (see Fig. 15) as follows:

\[ |m_j0⟩ = |e_{1j}⟩ \]  
\[ \text{and} \]
\[ e^{-im_j}U \downarrow |m_j0⟩ = \cos(ϕ_j)|e_{1j}⟩ + \sin(ϕ_j)|e_{2j}⟩ \]  
In the \( |e_{1j}⟩, |e_{2j}⟩ \) basis, we find after substituting \( m_j = e^{im_j} \cos(ϕ_j) \) into Eqs. (60) that

\[ W = \begin{bmatrix} \cos(2ϕ_j) & \sin(2ϕ_j) \\ -\sin(2ϕ_j) & \cos(2ϕ_j) \end{bmatrix} \]  

The eigenvalues of this matrix are \( e^{±i2ϕ_j} \), with corresponding eigenvectors:

\[ |ψ_{±j}⟩ = \frac{1}{\sqrt{2}}(|e_{1j}⟩ ± |e_{2j}⟩) \]  

These eigenvectors satisfy

\[ ⟨ψ_{−j}|ψ_{j}⟩ = 0 \quad ⟨ψ_{j}|ψ_{j}⟩ = 1 \]
By expressing $|e_1\rangle$ and $|e_2\rangle$ in Eq.(63) in the original basis, we get Eq.(59).

QED

Define the following vector spaces:

$$\mathcal{V} = \text{span}\{|x\rangle \otimes |y\rangle : x, y \in S_x\},$$  \hspace{2cm} (65)

$$\mathcal{V}_A = \text{span}\{|x\rangle \otimes |0\rangle : x \in S_x\},$$  \hspace{2cm} (66)

$$\mathcal{V}_B = U \downarrow \mathcal{V}_A,$$  \hspace{2cm} (67)

and

$$\mathcal{V}_{busy} = \mathcal{V}_A + \mathcal{V}_B.$$  \hspace{2cm} (68)

$\mathcal{V}$ can be expressed as a direct sum of $\mathcal{V}_{busy}$ and its orthogonal complement $\mathcal{V}_{busy}^\perp$:

$$\mathcal{V} = \mathcal{V}_{busy} \oplus \mathcal{V}_{busy}^\perp.$$  \hspace{2cm} (69)

From Claim 4, it follows that $\mathcal{V}_{busy}$ is a direct sum of the subspaces $\mathcal{V}_{busy}^j$:

$$\mathcal{V}_{busy} = \bigoplus_{j=0}^{N_S-1} \mathcal{V}_{busy}^j.$$  \hspace{2cm} (70)

Recall that matrices $M$ and $M_{sym}$ are $N_S$ dimensional whereas $W$ is $N_S^2$ dimensional. Since the size of $S_x$ is $N_S$, $\dim(\mathcal{V}) = N_S^2$. From Eq.(70) and Claim 4, $\dim(\mathcal{V}_{busy}) = 2N_S - 1$. Furthermore, $\{|\psi_j\rangle : j = 0, \pm 1, \pm 2, \ldots, \pm (N_S - 1)\}$ is an orthonormal basis for $\mathcal{V}_{busy}$.

At this point we’ve explained the action of $W$ on $\mathcal{V}_{busy}$, but we haven’t said anything about the action of $W$ on $\mathcal{V}_{busy}^\perp$. Next we show that $W$ acts simply as the identity on $\mathcal{V}_{busy}^\perp$. (This is what one would expect since the vectors in $\mathcal{V}_{busy}^\perp$ are parallel to the axis of the $W$ rotation.) Recall that if $S$ and $T$ are subspaces of a vector space $\mathcal{V}$, then $(S + T)^\perp = S^\perp \cap T^\perp$. Therefore,

$$\mathcal{V}_{busy}^\perp = \mathcal{V}^\perp_A \cap \mathcal{V}^\perp_B.$$  \hspace{2cm} (71)

From the definitions of $\mathcal{V}_A$ and $\mathcal{V}_B$, it’s easy to see that

$$\mathcal{V}_A^\perp = \text{span}\{|x\rangle \otimes |y\rangle : x \in S_x, \text{ and } y \in S_x - \{0\}\},$$  \hspace{2cm} (72)

and

$$\mathcal{V}_B^\perp = U \downarrow (\mathcal{V}_A^\perp).$$  \hspace{2cm} (73)
Claim 5

\[ W|\phi\rangle = |\phi\rangle \]

for all \(|\phi\rangle \in \mathcal{V}^\perp_{\text{busy}}\).

**Proof:** Let \(|\phi\rangle \in \mathcal{V}^\perp_{\text{busy}} = \mathcal{V}^\perp_A \cap \mathcal{V}^\perp_B\). Hence \(|\phi\rangle \in \mathcal{V}^\perp_A\) and \(|\phi\rangle = U \uparrow |\theta\rangle\) for some \(|\theta\rangle \in \mathcal{V}^\perp_A\).

\[
U(-1)^*U^\dagger(-1)^*|\phi\rangle = U \uparrow (-1)^\dagger \uparrow U^\dagger(-1)^0|\phi\rangle \tag{75a}
\]

\[
= U \uparrow (1 - 2\pi) \uparrow U^\dagger \uparrow |\theta\rangle \tag{75b}
\]

\[
= U \uparrow (1 - 2\pi)|\theta\rangle \tag{75c}
\]

\[
= |\phi\rangle . \tag{75d}
\]

QED

C.5 Multiplexor Implementation of \(W\)

Consider the case \(N_B = 2\). Using \(e^{i\pi} = -1\) and \(|0\rangle\langle 0| = \bar{n}\), one gets

\[
W = U(-1)^*U^\dagger(-1)^* =
\]

\[
U(-1)^*U^\dagger(-1)^* =
\]

\[
W = U(-1)^*U^\dagger(-1)^* =
\]

Now we need to find a SEO for the \(U\) in Eq. (76). Using Eq. (41) to express \(U\) in terms of \(\tilde{U}\), and using the method given in Appendix B for implementing \(\tilde{U}\) in terms of multiplexors, we get

\[
U = \uparrow \tilde{U}^\dagger \downarrow \tilde{U} =
\]

In Eq. (77), a box with a dagger in it represents the Hermitian conjugate of the box without a dagger and acting earlier on the same qubit. It’s clear how to generalize this construction of \(W\) to any number \(N_B\) of bits.

Figs. 16 and 17 show English and Picture files, written using the format of QuSAnn and Multiplexor Expander, for a Szegedy quantum walk operator \(W\), for a case with \(N_B = 2\).
D Appendix: Wocjan-Abeyesinghe Algorithm

In this appendix, we will review the Wocjan-Abeyesinghe Algorithm for quantum simulated annealing, for which QuSAnn generates a quantum circuit. This appendix follows closely Ref. [7].

For any inverse temperature $\beta > 0$, define $V_\beta$ by the quantum circuit of Fig.18. Fig.18 also defines the parameters $a = 1, 2, \ldots$ which we refer to as the number of probe bits, and $c = 1, 2, \ldots$ which we refer to as the number of phase estimation (PE) steps.

Let

$$Q = (e^{i\pi})^{a=0}$$

and

$$\tilde{R}_\beta = V_\beta^\dagger [I_2^{\otimes (2N_B)} \otimes Q] V_\beta .$$

(78)

(79)
Consider an annealing schedule $\beta_0, \beta_1, \ldots, \beta_{t_f}$. For each “time” $t \in \{0, 1, \ldots, t_f\}$, define a unitary matrix $U_{\beta_t:d_f}$ recursively as follows: Let

$$U_{\beta_t:0} = I_2^{\otimes (2N_B + ac)} ,$$

and

$$U_{\beta_t:d+1} = U_{\beta_t:d} \tilde{R}_{\beta_t} U_{\beta_t:d}^\dagger \tilde{R}_{\beta_{t+1}} U_{\beta_t:d} .$$

where $d \in \{0, 1, \ldots, d_f - 1\}$. See Fig. 19 for a pictorial representation of this recursion. We will call the parameter $d_f = 1, 2, \ldots$ which is the final level of recursion, the Grover depth.

If $\mathcal{U}$ is defined by

$$\mathcal{U} = U_{\beta_{f-1}:d_f} \cdots U_{\beta_2:d_f} U_{\beta_1:d_f} U_{\beta_0:d_f} ,$$

and if we’ve done things right, $\mathcal{U}$ should satisfy

$$\mathcal{U}|\sqrt{\pi_{\beta_0}} \otimes |0\rangle^{N_B} \otimes |0\rangle^{\otimes (ac)} \approx |\sqrt{\pi_{\beta_f}} \otimes |0\rangle^{N_B} \otimes |0\rangle^{\otimes (ac)} .$$
Figure 19: Pictorial representation of Grover recursion Eq.(80).

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