Supplementary Information

1 Formal Proof of the Search Complement Algorithm

In this section we provide a formal proof of the search complement algorithm.

To begin with, in Eq. (1) we provide the analytical form of an arbitrary fully controlled U gate with n top control qubits and m bottom target qubits

$$\mathscr{C}^n(U) = U \otimes |t\rangle\langle t| + I_2^{\otimes m} \otimes I_2^{\otimes n} - I_2^{\otimes m} \otimes |t\rangle\langle t| \tag{1}$$

$|t\rangle \in \mathbf{C}^n$ is the state that activates the target gate, U, and I_2 is the 2×2 identity. Notice that $\mathscr{C}^n$ acts as the identity whenever it is applied on a state $|i\rangle$ that is different from $|t\rangle$, but when the state is $|i\rangle = |t\rangle$, then the first and last term in Eq. (1) are activated, and the result is $U|t\rangle$.

The analytical form of the shift operator of the *CNOT* model to perform a UCDTQW on $\mathscr{K}_{2^n}$ is

$$S = \sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| \otimes |j\oplus i\rangle\langle j| \tag{2}$$

Once both shift and coin operators of the system are defined, let us obtain a reduced expression for the operator of the search complement algorithm, $\mathscr{U} = SC'(I_2^{\otimes n} \otimes H^{\otimes n})$, where n is the number of qubits of both position and coin registers.

$$\mathscr{U} = \left[\sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| \otimes |j\oplus i\rangle\langle j|\right]\left[H^{\otimes m} \otimes |t\rangle\langle t| + I_m \otimes I_m - I_m \otimes |t\rangle\langle t|\right]\left[I_2^{\otimes m} \otimes H^{\otimes n}\right]$$

$$\begin{aligned}\mathscr{U} = &\sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| H^{\otimes m} \otimes |j\oplus i\rangle\langle j|t\rangle\langle t| H^{\otimes n}\\ &+\sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| \otimes |j\oplus i\rangle\langle j| H^{\otimes n}\\ &-\sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| \otimes |j\oplus i\rangle\langle j|t\rangle\langle t| H^{\otimes n}\end{aligned} \tag{3}$$

Using the property $\langle j|t\rangle = \delta_{jt}$, $\mathscr{U}$ simplifies as follows

$$\begin{aligned}\mathscr{U} = &\sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| H^{\otimes m} \otimes |j\oplus i\rangle\,\delta_{jt}\,\langle t| H^{\otimes n}\\ &+\sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| \otimes |j\oplus i\rangle\langle j| H^{\otimes n}\\ &-\sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| \otimes |j\oplus i\rangle\,\delta_{jt}\,\langle t| H^{\otimes n}\end{aligned} \tag{4}$$

$$\begin{aligned}\Rightarrow \mathscr{U} = &\sum_{i=0}^{2^m-1} |i\rangle\langle i| H^{\otimes m} \otimes |t\oplus i\rangle\langle t| H^{\otimes n}\\ &+\sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| \otimes |j\oplus i\rangle\langle j| H^{\otimes n}\\ &-\sum_{i=0}^{2^m-1} |i\rangle\langle i| \otimes |t\oplus i\rangle\langle t| H^{\otimes n}\end{aligned} \tag{5}$$

Finally, we get

$$\mathscr{U} = \sum_{i=0}^{2^m-1} |i\rangle\langle i| \left(H^{\otimes m} - I_m\right) \otimes |t\oplus i\rangle\langle t| H^{\otimes n} + \sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i| \otimes |j\oplus i\rangle\langle j| H^{\otimes n} \tag{6}$$

Next, we use Eq. (6) to calculate the first step of the quantum walk. Consider the initial state of the quantum walk to be

$$|\psi_0\rangle = |r\rangle \otimes |s\rangle \tag{7}$$

Then

$$|\psi_1\rangle = \mathscr{U}\,|\psi_0\rangle \tag{8}$$

$$|\psi_1\rangle = \sum_{i=0}^{2^m-1} |i\rangle\langle i| \left(H^{\otimes m} - I_m\right)|r\rangle \otimes |t\oplus i\rangle\langle t| H^{\otimes n}|s\rangle + \sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i|r\rangle \otimes |j\oplus i\rangle\langle j| H^{\otimes n}|s\rangle \tag{9}$$

$$|\psi_1\rangle = \sum_{i=0}^{2^m-1} |i\rangle\langle i| H^{\otimes m}|r\rangle \otimes |t\oplus i\rangle\langle t| H^{\otimes n}|s\rangle - \sum_{i=0}^{2^m-1} |i\rangle\langle i|r\rangle \otimes |t\oplus i\rangle\langle t| H^{\otimes n}|s\rangle + \sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\langle i|r\rangle \otimes |j\oplus i\rangle\langle j| H^{\otimes n}|s\rangle \tag{10}$$

$$|\psi_1\rangle = \sum_{i=0}^{2^m-1} |i\rangle\langle i| H^{\otimes m}|r\rangle \otimes |t\oplus i\rangle\langle t| H^{\otimes n}|s\rangle - \sum_{i=0}^{2^m-1} |i\rangle\,\delta_{ir} \otimes |t\oplus i\rangle\langle t| H^{\otimes n}|s\rangle + \sum_{i=0}^{2^m-1}\sum_{j=0}^{2^n-1} |i\rangle\,\delta_{ir} \otimes |j\oplus i\rangle\langle j| H^{\otimes n}|s\rangle \tag{11}$$

Thus, the final expression for $|\psi_1\rangle$ is given by Eq. (12).

$$|\psi_1\rangle = \sum_{i=0}^{2^m-1} \langle i| H^{\otimes m}|r\rangle\langle t| H^{\otimes n}|s\rangle \Big(|i\rangle \otimes |t\oplus i\rangle\Big) - \langle t| H^{\otimes n}|s\rangle \Big(|r\rangle \otimes |t\oplus r\rangle\Big) + \sum_{j=0}^{2^n-1} \langle j| H^{\otimes n}|s\rangle \Big(|r\rangle \otimes |j\oplus r\rangle\Big) \tag{12}$$

Now, let us get the probability of finding the walker at an arbitrary position $|k\rangle$ when measured. For this, let us apply the measurement operator $M_k = I_m \otimes |k\rangle\langle k|$ to state $|\psi_1\rangle$.

$$M_k|\psi_1\rangle = \sum_{i=0}^{2^m-1} \langle i| H^{\otimes m}|r\rangle\langle t| H^{\otimes n}|s\rangle\langle k|t\oplus i\rangle \Big(|i\rangle \otimes |k\rangle\Big) - \langle t| H^{\otimes n}|s\rangle\langle k|t\oplus r\rangle \Big(|r\rangle \otimes |k\rangle\Big) + \sum_{j=0}^{2^n-1} \langle j| H^{\otimes n}|s\rangle\langle k|j\oplus r\rangle \Big(|r\rangle \otimes |k\rangle\Big) \tag{13}$$

$$
\begin{aligned}
\Rightarrow M_k \left|\psi_1\right\rangle = &\sum_{i=0}^{2^m-1} \langle i| H^{\otimes m} |r\rangle \langle t| H^{\otimes n} |s\rangle \, \delta_{k,t\oplus i} \Big(|i\rangle \otimes |k\rangle \Big) \\
&- \langle t| H^{\otimes n} |s\rangle \, \delta_{k,t\oplus r} \Big(|r\rangle \otimes |k\rangle \Big) \\
&+ \sum_{j=0}^{2^n-1} \langle j| H^{\otimes n} |s\rangle \, \delta_{k,j\oplus r} \Big(|r\rangle \otimes |k\rangle \Big)
\end{aligned} \tag{14}
$$

Now, in order to contract the Kronecker deltas in the last expression and to facilitate calculations, consider two integers u and v such that

$$k = t \oplus u \tag{15}$$

$$k = v \oplus r \tag{16}$$

This allows us to turn Eq. (14) into

$$
\begin{aligned}
M_k \left|\psi_1\right\rangle = &\langle u| H^{\otimes m} |r\rangle \langle t| H^{\otimes n} |s\rangle \Big(|u\rangle \otimes |k\rangle \Big) \\
&+ \big(\langle v| H^{\otimes n} |s\rangle - \delta_{k,t\oplus r} \langle t| H^{\otimes n} |s\rangle \big) \Big(|r\rangle \otimes |k\rangle \Big)
\end{aligned} \tag{17}
$$

The probability is then given by the squared modulus of this expression, i.e.

$$
\begin{aligned}
\Rightarrow |M_k \left|\psi_1\right\rangle|^2 = &\big(\langle u| H^{\otimes m} |r\rangle \big)^2 \big(\langle t| H^{\otimes n} |s\rangle \big)^2 \\
&+ \big(\langle v| H^{\otimes n} |s\rangle - \delta_{k,t\oplus r} \langle t| H^{\otimes n} |s\rangle \big)^2
\end{aligned} \tag{18}
$$

$$\tag{19}$$

$$
\begin{aligned}
|M_k \left|\psi_1\right\rangle|^2 = &\big(\langle u| H^{\otimes m} |r\rangle \big)^2 \big(\langle t| H^{\otimes n} |s\rangle \big)^2 \\
&+ \big(\langle v| H^{\otimes n} |s\rangle \big)^2 + \delta_{k,t\oplus r} \big(\langle t| H^{\otimes n} |s\rangle \big)^2 \\
&- \delta_{k,t\oplus r} \langle t| H^{\otimes n} |s\rangle \langle v| H^{\otimes n} |s\rangle
\end{aligned} \tag{20}
$$

Notice then that $\langle a| H^{\otimes m} |b\rangle$ is the (a,b)-th entry in the m dimensional Hadamard matrix. That is,

$$\langle a| H^{\otimes m} |b\rangle = \frac{(-1)^{a\cdot b}}{\sqrt{2^m}} \tag{21}$$

where $a \cdot b$ is the *binary dot product* or the number 1 bits a and b have in common in their binary representations. Notice then that the value of $a \cdot b$ does not matter when obtaining the square of the entry

$$\big(\langle a| H^{\otimes m} |b\rangle \big)^2 = \frac{1}{2^m} \tag{22}$$

This turns Eq. (20) into

$$p_k = \left(\frac{1}{2^m}\right)\left(\frac{1}{2^n}\right) + \frac{1}{2^n} + \frac{\delta_{k,t\oplus r}}{2^n} - \delta_{k,t\oplus r} \langle t| H^{\otimes n} |s\rangle \langle v| H^{\otimes n} |s\rangle \tag{23}$$

Which is the general expression for the probability of measuring a node using the search complement algorithm.

Notice that we still have one Kronecker delta left, which leaves us with two cases.

1. Case 1: When $k \neq t \oplus r$

   The probability of measuring the state associated to node k is

$$p(v_k) = \frac{1}{2^{m+n}} + \frac{1}{2^n} \tag{24}$$

2. Case 2: When $k = t \oplus r$

   The probability of measuring the state associated to node k is

$$p(v_k) = \frac{1}{2^{m+n}} + \frac{1}{2^n} + \frac{1}{2^n} - 2\langle t| H^{\otimes n} |s\rangle \langle v| H^{\otimes n} |s\rangle \tag{25}$$

Moreover, as v is defined by $k = v \oplus r$ and $k = t \oplus r$, we must have $v = t$, and thus:

$$\begin{aligned} p(v_k) &= \frac{1}{2^{m+n}} + \frac{2}{2^n} - 2\big(\langle t| H^{\otimes n} |s\rangle\big)^2 \\ &= \frac{1}{2^{m+n}} + \frac{2}{2^n} - \frac{2}{2^n} \\ &= \frac{1}{2^{m+n}} \end{aligned}$$

Lastly, given that the coin state is represented with the same number of bits as the position state in $|\psi\rangle$, that is $m = n$, we get the following final expression for the probability distribution of a quantum walker:

$$p(v_k) = \begin{cases} \frac{1}{4^n} & \text{if } k = t \oplus r \\ \frac{1}{4^n} + \frac{1}{2^n} & \text{if } k \neq t \oplus r \end{cases} \tag{26}$$

In the case where $|r\rangle = |0\rangle$, then the probability of measuring the target state is $p(v_t) = \frac{1}{4^n}$, while the probability of measuring any other state is $p(v_{k \neq t}) = \frac{1}{4^n} + \frac{1}{2^n}$. Thus, the probability of measuring the target state $|t\rangle$ is indeed minimized.

To prove that Eq. (26) is indeed a probability distribution we calculate the sum of all probabilities, i.e.

$$\sum_{i=0}^{2^n-1} p(v_i) = p(v_{t\oplus r}) + \sum_{i \neq t \oplus r} p(v_i)$$

Given that there are $2^n - 1$ non-target states, we get

$$\sum_{i=0}^{2^n-1} p(v_i) = \frac{1}{4^n} + \left(2^n - 1\right)\left(\frac{1}{4^n} + \frac{1}{2^n}\right) = \frac{1}{4^n} + \left(\frac{1}{2^n} + 1\right) - \left(\frac{1}{4^n} + \frac{1}{2^n}\right)$$

$$\therefore \sum_{i=0}^{2^n-1} p(v_i) = 1$$

2 Calibration Data

In this section we provide the calibration parameters of the quantum processor imbq_manila at the time of running the search complement algorithm to obtain the experimental data for Figure 14 and Table 1 in the main text.

Table 1. Calibration of quantum processor imbq_manila when executing the search complement algorithm. The results of the algorithm are shown in Figure 14 and Table 1 of the main text.

Qubit/Parameter	Q_0	Q_1	Q_2	Q_3	Q_4
$T_1(\mu s)$	149.09	203.7	161.46	203.01	108.82
T_2 (μs)	90.93	87.48	22.82	58.99	17.28
Frequency (GHz)	4.963	4.838	5.037	4.951	5.066
Anhamonicity (GHz)	-0.34335	-0.34621	-0.34366	-0.34355	-0.34211
Readout assignment error (10^{-2})	2.05	1.71	1.99	1.95	2.09
Prob meas0 prep1	0.0306	0.152	0.03	0.0256	0.0316
Prob meas1 prep0	0.0104	0.1902	0.0098	0.0134	0.0102
Readout length (ns)	5351.111	5351.111	5351.111	5351.111	5351.111
ID error (10^{-4})	1.83	6.84	3.18	2.09	4.19
$\sqrt{x}$ error (10^{-4})	1.83	6.84	3.18	2.09	4.19
Single-qubit Pauli-X error (10^{-4})	1.83	6.84	3.18	2.09	4.19
CNOT error (10^{-2})	0-1:1.335	1-2:1.715; 1-0:1.335	2-3:1.126; 2-1:1.715	3-4:0.5390; 3-2:1.126	4-3:0.5390
Gate time (ns)	0-1:277.333	1-2:469.333; 1-0:312.889	2-3:355.556; 2-1:504.889	3-4:334.222; 3-2:391.111	4-3:298.667