Schumacher’s quantum data compression
as a quantum computation

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Abstract

An explicit algorithm for performing Schumacher’s noiseless compression of quantum bits is given. This algorithm is based on a combinatorial expression for a particular bijection among binary strings. The algorithm, which adheres to the rules of reversible programming, is expressed in a high-level pseudocode language. It is implemented using \(O(n^3)\) two- and three-bit primitive reversible operations, where \(n\) is the length of the qubit strings to be compressed. Also, the algorithm makes use of \(O(n)\) auxiliary qubits; however, space-saving techniques based on those proposed by Bennett are developed which reduce this workspace to \(O(\sqrt{n})\) while increasing the running time by
less than a factor of two.

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I. INTRODUCTION

There is considerable interest in the controlled generation, manipulation and transportation of individual quantum states; applications of such resources are envisioned in new kinds of data transmission, cryptography and computation. The quantum extension of conventional bits, called *qubits*, have been subject to considerable exploration lately. A single qubit is embodied in the state of a single two-state quantum system, such as the spin degree of freedom of an electron or other spin-$\frac{1}{2}$ particle, where the spin-up state of the particle is denoted by $|0\rangle$ and the spin-down state is denoted by $|1\rangle$. The basic laws of quantum physics dictate that a description of the entire possible state-space of the qubit is given by

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

where $\alpha$ and $\beta$ are any two complex numbers such that $|\alpha|^2 + |\beta|^2 = 1$. This is called a “qubit” since it can assume one of two binary values, but of course it has fundamentally different properties because of the possibility of it being in a superposition of these two values. The properties with which quantum mechanics endows the qubit make possible a kind of cryptography which is fundamentally secure against eavesdropping attacks [1], and computations which apparently violate the complexity-class categorizations for ordinary boolean computers [2].

One of the ideas of this sort that has been understood recently is the possibility of data compression for qubits. In classical information theory, if $n$ bits, $x_1, \ldots, x_n$, are each sampled independently according to some probability distribution $p = (p_0, p_1)$ (on the set $\{0, 1\}$) then the string $x_1 \ldots x_n$ may be compressed to a $nH_s(p)$-bit string (where $H_s(p) = -\sum_{i=0}^{1} p_i \log p_i$, the Shannon entropy [3])—and no further—in the following asymptotic sense. For any $\varepsilon, \delta > 0$, for sufficiently large $n$, for any $\lambda(n) \geq n(H_s(p) + \delta)$, $\lambda(n) \in \{1, \ldots, n\}$, there exists a compression scheme that compresses $x_1 \ldots x_n$ to $y_1 \ldots y_{\lambda(n)}$, and such that $x_1 \ldots x_n$ can be successfully recovered from $y_1 \ldots y_{\lambda(n)}$ with probability greater than $1 - \varepsilon$. Moreover, the
above compression is the maximum possible in the sense that, for any \( \varepsilon, \delta > 0 \), for sufficiently large \( n \), for any \( \lambda(n) \leq n(H_\mathbb{S}(p) - \delta) \), for any compression scheme that maps \( x_1 \cdots x_n \) to \( y_1 \cdots y_{\lambda(n)} \), the probability that \( x_1 \cdots x_n \) can be successfully recovered from \( y_1 \cdots y_{\lambda(n)} \) is less than \( \varepsilon \).

The quantum physical analogue of the above scenario involves the compression of a string of qubits, instead of bits. Note that there are a continuum of possible states for each qubit, rather than two possible values. We shall consider the “discrete” case, where a probability distribution is concentrated on some finite set of qubit states \( \mathcal{S} = \{ |\Psi_1\rangle, \ldots, |\Psi_m\rangle \} \). Let the respective probabilities be \( p = (p_1, \ldots, p_m) \). In the language of quantum physics, \((\mathcal{S}, p)\) defines an ensemble of states. Let \( |\alpha_1\rangle \cdots |\alpha_n\rangle \) be a string of \( n \) qubits, each sampled independently from \((\mathcal{S}, p)\). Define a compressor \( A \) as a unitary transformation that maps \( n \)-qubit strings to \( n \)-qubit strings. Again let \( \lambda(n) \in \{1, \ldots, n\} \). It is to be understood that, on input \( |\alpha_1\rangle \cdots |\alpha_n\rangle \), the first \( \lambda(n) \) qubits that are output by the compressor \( |\beta_1 \cdots \beta_{\lambda(n)}\rangle \) are taken as the compressed version of its input, and the remaining \( n - \lambda(n) \) qubits are discarded. A decompressor \( B \) is a unitary transformation that maps \( n \)-qubit strings to \( n \)-qubit strings. It is to be understood that the first \( \lambda(n) \) qubits input to the decompressor are \( |\beta_1 \cdots \beta_{\lambda(n)}\rangle \), the compressed version of some sequence of \( n \) qubits, and the remaining \( n - \lambda(n) \) qubits are all \( |0\rangle \). An \( n \)-to-\( \lambda(n) \) quantum compression scheme is a compressor/decompressor pair \((A, B)\). As in the classical case, the goal is to achieve as high a compression rate (i.e. as small a \( \lambda(n) \)) as possible, while permitting the original message to be recovered from its compressed version, with high probability.

Assume that the compressor knows (i.e. can be a function of) the underlying ensemble \((\mathcal{S}, p)\), but has no explicit knowledge about the specific random selections made (interestingly, compressors exist that know even less than \((\mathcal{S}, p)\); more about this later). In the classical case, the compressor obtains complete information about the bits to be compressed, but complete information cannot generally be obtained from a qubit. If the possible qubit states in \( \mathcal{S} \) are not mutually orthogonal then any observation of such a qubit will only yield partial information about its state, and can irretrievably change this state. Due to this,
one might expect to be able to achieve less in the quantum scenario than with classical compression schemes — in fact, the opposite is true.

Let us measure the quality of an $n$-to-$\lambda(n)$ compression scheme $(A, B)$ with respect to a source distribution $p$ in terms of its fidelity, defined as follows. Consider the following experiment. Let the sequence $|\alpha_1\rangle \ldots |\alpha_n\rangle$ be sampled independently from $(S, p)$. Transform $|\alpha_1\rangle \ldots |\alpha_n\rangle$ according to the compressor $A$ and let $|\beta_1\ldots\beta_\lambda(n)\rangle$ be the compressed version. Next, transform $|\beta_1\ldots\beta_\lambda(n)\rangle|0\ldots0\rangle$ according to the decompressor $B$ and let $|\alpha'_1\ldots\alpha'_n\rangle$ be the output. Finally, measure $|\alpha'_1\ldots\alpha'_n\rangle$ with respect to a basis containing $|\alpha_1\ldots\alpha_n\rangle$. The fidelity is the probability $|\langle\alpha'_1\ldots\alpha'_n|\alpha_1\ldots\alpha_n\rangle|^2$ that this measurement results in $|\alpha_1\ldots\alpha_n\rangle$.

Note that the fidelity is with respect to two sources of randomness: (a) the random choices in the original generation of $|\alpha_1\ldots\alpha_n\rangle$; and (b) the randomness that results from performing a measurement of the state $|\alpha'_1\ldots\alpha'_n\rangle$. Roughly speaking, the fidelity can be high if for “most” choices in (a), $|\alpha'_1\ldots\alpha'_n\rangle$ is “close to” $|\alpha_1\ldots\alpha_n\rangle$.

The ensemble $(S, p)$ represents a mixed state, which has density matrix $\rho$, defined as

$$
\rho = \sum_{i=1}^{m} p_i |\Psi_i\rangle \langle \Psi_i|.
$$

The von Neumann entropy corresponding to $(S, p)$ is defined in terms of the density matrix $\rho$ as $H_{VN}(\rho) = -\text{Tr}(\rho \log \rho)$. In general, $H_{VN}(\rho) \leq H_S(p)$, with equality occurring if and only if the states in $S$ are mutually orthogonal.

Roughly speaking, Schumacher’s theorem [4] states that $nH_{VN}(\rho)$ is asymptotically the maximum compression attainable for $n$ qubits resulting from a source with density matrix $\rho$. More precisely, let $(S, p)$ be any ensemble of qubits, and $\rho$ be the corresponding density matrix. Then, for all $\varepsilon, \delta > 0$, for sufficiently large $n$ and $\lambda(n) \geq n(H_{VN}(\rho) + \delta)$, there exists an $n$-to-$\lambda(n)$ quantum compression scheme for $(S, p)$ with fidelity greater than $1 - \varepsilon$. Moreover, for all $\varepsilon, \delta > 0$, for sufficiently large $n$, if $\lambda(n) \leq n(H_{VN}(\rho) - \delta)$ then every $n$-to-$\lambda(n)$ quantum compression scheme has fidelity less than $\varepsilon$.

It should be noted that the above bounds are robust in the sense that they do not change when a number of technical variations are made in the scenario. For example, the $n$-to-$\lambda(n)$
compression schemes that attain fidelity greater than $1 - \varepsilon$ can restricted to being highly “oblivious” in that they depend only on knowing a basis for which the density matrix is diagonal, with nonincreasing values along the diagonal. Also, even if the compressor is supplied with complete information about the state of the source string $|\alpha_1 \ldots \alpha_m\rangle$ that it receives, $\varepsilon$ still bounds the fidelity attainable if $\lambda(n) \leq n(H_{VN}(\rho) - \delta)$.

The proof of Schumacher’s Theorem is based on the existence of a “typical subspace” $\Lambda$ of the Hilbert space of $n$ qubits, which has the property that, with high probability, a sample of $|\alpha_1, \ldots, \alpha_n\rangle$ has almost unit projection onto $\Lambda$. It has been shown that the dimension of $\Lambda$ is $2^{nH_{VN}(\rho)}$; thus, the operation that the compressor should perform involves “transposing” the subspace $\Lambda$ into the Hilbert space of a smaller block of $nH_{VN}(\rho)$ qubits.

Bennett gives a more explicit procedure for accomplishing this “transposition”, which we illustrate with an example. Suppose that $S = \{|\Psi_1\rangle, |\Psi_2\rangle\}$, where $|\Psi_1\rangle = |0\rangle$ and $|\Psi_2\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$, and $p = (p_1, p_2)$, where $p_1 = p_2 = \frac{1}{2}$. The density matrix corresponding to $(S, p)$ is $\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle)(\frac{1}{\sqrt{2}}\langle 0| + \frac{1}{\sqrt{2}}\langle 1|)$, or, in $2 \times 2$ matrix form,

$$
\rho = \begin{pmatrix}
\frac{3}{4} & 1 \\
\frac{1}{4} & \frac{1}{4}
\end{pmatrix}
$$

in the basis $|0\rangle$.

It is always possible to go to a basis in which the density matrix is diagonal:

$$
\rho' = \begin{pmatrix}
\lambda_{\text{max}} & 0 \\
0 & \lambda_{\text{min}}
\end{pmatrix}
= \begin{pmatrix}
\frac{3}{4} + \frac{1}{4} \tan \frac{\pi}{8} & 0 \\
0 & \frac{1}{4} - \frac{1}{4} \tan \frac{\pi}{8}
\end{pmatrix}
$$

in the basis $|0'\rangle = \cos \frac{\pi}{8}|0\rangle + \sin \frac{\pi}{8}|1\rangle$ and $|1'\rangle = -\sin \frac{\pi}{8}|0\rangle + \cos \frac{\pi}{8}|1\rangle$.

Both of the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ have large overlap on the basis state $|0'\rangle$ ($|\langle \Psi_i|0'\rangle| = \cos \frac{\pi}{8}$), and small overlap on the orthogonal basis state $|1'\rangle$ ($|\langle \Psi_i|1'\rangle| = \sin \frac{\pi}{8}$). This observation leads to a way of compressing strings of signal states. Consider all $n$-qubit strings possible from the states in $S$. These strings can all be expressed with respect to the basis consisting of $|x_{n-1} \ldots x_0\rangle = |x_{n-1}\rangle \ldots |x_0\rangle$, where $x_{n-1}, \ldots, x_0 \in \{0', 1'\}$. Each such $|x_{n-1} \ldots x_0\rangle$ can be interpreted as an $n$-bit binary number, and, thus, can be denoted as $|x\rangle$, for $x \in$
\{0, \ldots, 2^n - 1\}. Now, the overlap of \(|x\rangle\) with the states in \(S^n\) is \(|\langle x|S^n\rangle| = \cos^m \frac{\pi}{8} \sin^{n-m} \frac{\pi}{8}\), where \(m\) is the number of 0’s in the binary representation of \(x\). Because this overlap diminishes exponentially with \(n - m\), basis states with large numbers of 1’s are relatively unimportant for describing any string \(|\alpha_1, \ldots, \alpha_n\rangle\); the Hilbert space can thus be truncated to the typical subspace \(\Lambda\) consisting of all states \(|x\rangle\) in which the binary number \(x\) contains a proportion of 1’s less than \(H_{\nu\nu}(\rho) < 0.601\).

Thus the “transposition” which the coder must do consists of mapping this \(\Lambda\) subspace for \(n\) qubits into the states spanned by less than 0.601\(n\) of those qubits.

We must accomplish this by a unitary transformation applied to the original states of the \(n\) qubits. In the basis \(|0\rangle, \ldots, |2^n - 1\rangle\), this transformation must map qubit strings with the smallest number of 1’s in succession into qubit binary strings with the smallest numerical value. This is a classical combinatorial calculation, “classical” in the sense that definite binary-number states are mapped to other definite binary-number states; however, it is essential that the computation be performed quantum mechanically, since the computation must preserve the superpositions of these basis states. This means that the combinatorial computation must be performed using reversible, quantum-coherent elementary operations.

The principal object of this paper is to derive the quantum computation which is needed to do this Schumacher coding. In Sec. II we derive the analytical formula for the sorting calculation required for the coding. Sec. III constructs the quantum program for performing this calculation: Sec. IIIA illustrates a first attempt at this coding exercise; Sec. IIIB discusses the way in which the calculation is to be properly made reversible; and Sec. IIIC, which contains the essential result of the paper, gives the final quantum program for Schumacher coding. Sec. IV gives, in the same programming notation developed in the earlier sections, the bit-level routines needed for performing the steps in the high-level program. Appendix A discusses how these bit-level routines may be made highly space-efficient, with only a modest increase in running time (these latter routines result in a smaller time-space product, which may be desirable [7,8]). Appendix B provides other ways of economizing in the bit-level implementation of these codes, by using some of the phase freedom coming
from the quantum-mechanical nature of the computation.

II. COMBINATORIAL EXPRESSION FOR SCHUMACHER CODING

As Bennett [6] has described, a specific realization of the unitary transformation performing the Schumacher coding function on a set of identical qubits consists of a sorting computation in which the states $|0\rangle, \ldots, |2^n - 1\rangle$ are given a lexicographical ordering according to how many 1’s are in their binary expansion. So, $|0\rangle$ is mapped to itself, all the states containing exactly one 1 and $n - 1$ 0’s are mapped to the states between $|1\rangle$ and $|n\rangle$, all the states with exactly two 1’s and $n - 2$ 0’s are mapped to the states between $|n + 1\rangle$ and $|n + n(n - 1)/2\rangle$, and, in general, all the states with exactly $m$ 1’s and $n - m$ 0’s are mapped to the states between

$$|\sum_{i=0}^{m-1} \binom{n}{i}\rangle$$

and

$$|\sum_{i=0}^{m} \binom{n}{i} - 1\rangle$$

inclusive. The Schumacher function does not require any particular ordering of the states within each of these blocks, except that the mapping must be 1-to-1 (i.e., a bijection); but, it turns out to be convenient to preserve lexicographical ordering within each block. Defining the index number within each block as $I[x, n, m]$, the total Schumacher function for string $x$ (with $n$ bits and $m$ 1’s) is

$$y = \sum_{i=0}^{m-1} \binom{n}{i} + I[x, n, m].$$

The index number $I$ obeys a recursive relationship which we now derive. Considering the possible binary-number strings representing the input state $x$, any string whose first 1 occurs in the $p + 1$st place (i.e., whose first $p$ bits are 0) must have a higher index number than all strings in which the first $p + 1$ places are 0. There are exactly $\binom{n-p+1}{m}$ such strings. This means that for the particular input string
\[ x = 00 \ldots 001000 \ldots 001111 \ldots 1, \]

the index number \( I[x, n, m] = \binom{n-p-1}{m} \). This result permits the index number of the more complex string

\[ x = 00 \ldots 001 \underbrace{x'}_{n-p-1 \text{ bits}} \]

(8)

to be expressed recursively:

\[ I[x, n, m] = \binom{n-p-1}{m} + I[x', n-p-1, m-1]. \]

(9)

It is probably easiest to understand Eq. (9) by writing out an example:

\[
\begin{align*}
I[0010011011, 10, 5] &= \binom{10-2-1}{5} + I[0011011, 7, 4] \\
&\downarrow \\
&\binom{7-2-1}{4} + I[1011, 4, 3] \\
&\downarrow \\
&\binom{4-0-1}{3} + I[011, 3, 2] \\
&\downarrow \\
&0.
\end{align*}
\]

(10)

As this illustrates, the recursion of Eq. (9) may be iterated to produce an expression for \( I \) for a general input string \( x \):

\[ I[x, n, m] = \sum_{i=1}^{n-1} x_{n-i} \left( \frac{n-i}{\sum_{k=1}^{n} x_{n-k}} \right). \]

(11)

Here the notation \( x_p \) denotes the value of the \( p^{th} \) bit of the string \( x \). Combining Eq. (11) with Eq. (6) yields the final expression for the Schumacher coding function:

\[ y = \sum_{k=0}^{n-1} x_k \binom{n}{i} + \sum_{j=1}^{n-1} x_j \left( \frac{j}{\sum_{k=0}^{j} x_k} \right). \]

(12)

In this equation, binary coefficients outside their natural range (e.g., \( \binom{n}{n+1} \)) are understood to be zero.
III. HIGH-LEVEL QUANTUM PROGRAM FOR SCHUMACHER CODING

A. first attempts

It is now our object to translate Eq. (12) into a sequence of elementary quantum-mechanical manipulations. We proceed to do this by writing out the calculation in a high-level “pseudocode” which, when “compiled”, would permit the operation to be performed by a sequence of elementary spectroscopic manipulations such as two-bit XOR’s (or controlled-NOT’s), along with one-bit rotations. Rather than building up the rules of this pseudocode axiomatically, we will proceed in an intuitive fashion. The principal constraint which the coded calculation must obey is that it be done reversibly. Instead of going into a discourse about this, let us present the first try at coding Eq. (12) (not a perfectly successful one, in fact):

Program FIRST_TRY

quantum registers:

\( X \) : \( n \)-bit register
\( Y \) : \( n \)-bit arithmetic register (initialized to 0)
\( S \) : \( \lceil \log n \rceil \)-bit arithmetic register (initialized to 0)

if \( X_0 = 1 \) then \( S \leftarrow S + 1 \)
for \( j = 1 \) to \( n - 1 \) do
  if \( X_j = 1 \) then \( S \leftarrow S + 1 \)
  for \( m = 0 \) to \( j + 1 \) do
    if \( X_j = 1 \) and \( S = m \) then \( Y \leftarrow Y + \binom{j}{m} \)
  for \( i = 0 \) to \( n - 1 \) do
    if \( i + 1 \leq S \) then \( Y \leftarrow Y + \binom{n}{i} \)

FIRST_TRY is not incorrect, but it is incomplete, in ways which we will repair by stages below. Here are some rules of this programming: All the quantum-mechanical registers are in capital letters. In FIRST_TRY, these are \( X \) (which is initialized with an input state \( x \), or a quantum superposition of such input states), \( Y \) (which is initialized to 0, and whose final value is the output state \( y \) or their quantum superpositions), and \( S \) (a small work register, also initialized to 0). The notation \( X_i \) indicates the \( i \)-th bit of \( X \). Note that \( Y \)
and $S$ are given the data type “arithmetic”, indicating that ordinary integer addition and subtraction are allowed with them. Only bitwise manipulations are performed on $X$. (In the **FINAL_SCHUMACHER** program, both bitwise and arithmetic manipulations will be performed on the same registers.)

All other lower-case variables in the program always have definite values and can (and should) be implemented using classical bits. Only the quantum registers need to be explicitly treated reversibly. So, the binomial coefficients $\binom{j}{m}$ can be precomputed or evaluated by any means, reversible or not, in the implementation of the quantum computation.

In a reversible program statement, the input can always be deduced from the output. So, for example, the statement

$$\textbf{if } X_0 = 1 \textbf{ then } S \leftarrow S + 1$$

is reversible, because the input could be deduced by the “time-reverse” of this statement,

$$\textbf{if } X_0 = 1 \textbf{ then } S \leftarrow S - 1$$

An irreversible program statement would be

$$\textbf{if } X_0 = 1 \textbf{ then } S \leftarrow 1$$

since the prior value of $S$ cannot be deduced. As it happens, this statement would function correctly in **FIRST_TRY** because $S$ actually is equal to 0 at this first executable statement of the program. However, we will enforce a rule that the only irreversible statements permitted that involve quantum variables will be the “initialized” designations present in the declaration statements. In later programs we will introduce a “finalized” designation, which will merely serve as a reminder that certain variables will always end the program with a particular value if the program runs correctly. This designation will be an important one in constructing reversible code. It is also a reminder that physically, the finalization can serve as a useful check that no error has occurred; a quantum measurement of this register at the end of the running of program should always find the register in the finalized value.

One further comment about the program statement

$$\textbf{if } X_0 = 1 \textbf{ then } S \leftarrow S + 1.$$  

If $S$ were a one-bit variable, this statement would just be a quantum XOR or controlled
NOT, in which the value of $S$ is inverted conditional on the value of $X_0$. In **FIRST_TRY**, $S$ is a multibit register, in fact it must have about $\log_2 n$ bits. Implementation of these multi-bit functions in terms of primitive operations involving no more than three bits is straightforward, and is presented in Sec. [V] and in Ref. [12,13]. Using quantum gates, all the three-bit primitives may be reduced to sequences of two-bit operations [10].

A few more points about **FIRST_TRY** are in order. Given the constraints of reversibility, it is a relatively straightforward transcription of Eq. (12). The first for loop (indexed by $j$) implements the second term of Eq. (12); this is efficient because the partial sum in the binomial coefficient can be accumulated in $S$ one term at a time, and then the completed sum can be used as the upper limit of the first term of (12), which is implemented in the second for loop. This inner $m$ loop could be replaced by the single statement

$$\text{if } X_j = 1 \text{ then } Y \leftarrow Y + \binom{j}{S},$$

but this would require a reversible calculation of the binomial function; we have chosen to make this binomial-coefficient calculation classical by writing out the loop as shown. One might also be tempted to modify the inner loop as follows:

$$\text{if } X_j = 1 \text{ then}
\begin{align*}
\text{for } m = 0 \text{ to } j + 1 \text{ do} \\
\text{if } S = m \text{ then } Y \leftarrow Y + \binom{j}{m}
\end{align*}$$

While moving the if statement from the loop is superficially more efficient, it turns out that, when these statements are re-expressed in terms of primitive operations, the if must be carried down to the lowest level in any case; so, we prefer a syntax in which such conditionals are explicitly shown at the lowest level.

**B. Reversibility considerations**

Now, what is the overall effect of **FIRST_TRY**, and why is it inadequate for performing the Schumacher function? Let $f : \{0,1\}^n \rightarrow \{0,1\}^n$ denote the Schumacher function for $n$-bit binary strings. If the total input state is expressed as the ket
\[ |X, Y, S\rangle = |x, 0, 0\rangle, \quad (13) \]

then the complete final state is
\[ |X, Y, S\rangle = |x, f(x), s\rangle, \quad (14) \]

(where \( s \) is the number of 1’s in \( x \)). But, the correct Schumacher function must have a final state of the form
\[ |X, Y, S\rangle = |0, f(x), 0\rangle. \quad (15) \]

That is, the input \( x \) should be erased and the work register \( S \) should be reset to its initial value of 0. This is possible to accomplish reversibly because the Schumacher function is bijective, so that no record of the initial state, or of the state of the work bits, needs to be retained at the end; they are completely deducible from the output. In fact, the correct operation of the Schumacher function requires that the output be of the form (14): if it is of the form of (14), then the final state is “entangled” with the initial state, which means that output states cannot be placed in the desired superpositions of states. Thus, the net result of the Schumacher function should be confined to the input data register only; this condition is obtainable from Eq. (15) if the final output state is swapped so that the state vector becomes
\[ |X, Y, S\rangle = |f(x), 0, 0\rangle. \quad (16) \]

Thus the Schumacher function is applied, “in-place”, to the first \( n \) qubits, while the remaining \( n + \log_2 n \) bits return to their original states, and may all be viewed simply as work space for the computation. We will see later that the “output” register \( Y \) can actually be removed entirely by using some clever programming. Some other workspace, not displayed explicitly in (16), appears to be necessary to do the bit-level manipulations in the Schumacher function (see Sec. IV); Appendix A shows that the size of this extra workspace does not have to exceed about \( 2\sqrt{n} \) bits.
These considerations have arisen previously in the context of reversible programming [14], but the rationale for constructing a function in the “fully-reversible” manner as specified by the output state (16) is somewhat different than in the classical context. In traditional reversible programming the object is to avoid the small energy cost involved in irreversible erasure of any of the working bits in the computer. If such an erasure is performed, the result of the computation will still be correct, even though the desired goal of expending no energy is not achieved. But in quantum computation, irreversible erasure of the state of register $X$ in Eq. (14) actually causes register $Y$ to be in the wrong quantum state, in so far that, if the initial $X$ was in a superposition of computational states, the final state of $Y$ will be a mixed quantum state, rather than the intended, pure superposition state. Thus, the consequences of irreversibility are more serious than in conventional reversible computation.

A method for designing a calculation to arrive at the desired final states (15) or (16), as already worked out in the earlier literature [14], requires two steps: 1) zero out $S$ and any other workspaces used by the program, and 2) explicitly implement the inverse of the Schumacher function Eq. (12). This can be accomplished by a program that, on input state

$$|X, Y, S\rangle = |x, y, 0\rangle,$$

produces the final state

$$|X, Y, S\rangle = |x \oplus f^{-1}(y), y, 0\rangle.$$

Note that applying such a transformation to the state

$$|X, Y, S\rangle = |x, f(x), 0\rangle$$

yields the required state

$$|X, Y, S\rangle = |0, f(x), 0\rangle.$$

Eq. (18) is not implemented simply by running FIRST_TRY in reverse; indeed, the inverse function can have very different and much greater complexity than the function itself.
Fortunately, in this case, as we will see in a moment, the inverse Schumacher function is also relatively easy to implement.

Step (1) above, zeroing out \( S \), is readily performed by adding code to the end of `FIRST_TRY` to simply subtract away the bits which have been added to \( S \):

```plaintext
for j = 0 to n - 1 do
    if \( X_j = 1 \) then \( S \leftarrow S - 1 \)
```

This code, added to the end of `FIRSTTRY`, produces the output state (19).

Step (2) above, implementing the inverse function Eq. (18), requires a new algorithm. We have not found any way to write the inverse Schumacher coding function as a formula as in Eq. (12). Nevertheless, a straightforward algorithm can be deduced from the following two inequalities. The first is obtained by combining the information from Eqs. (4) and (5):

\[
\sum_{i=0}^{m-1} \binom{n}{i} \leq y < \sum_{i=0}^{m} \binom{n}{i},
\]

(21)

where

\[
m = \sum_{k=0}^{n-1} x_k
\]

(22)

is the number of 1’s in the binary string \( x \). We will be able to write simple pseudocode to compute \( m \) (a.k.a. \( S \)). This result can then be used to compute \( I[x, n, m] \) using Eq. (6). \( I[x, n, m] \) satisfies an inequality which is a simple consequence of Eq. (4) and the discussion preceding it:

\[
\binom{n-p-1}{m} \leq I[x, n, m] < \binom{n-p}{m}.
\]

(23)

By finding the \( p \) which satisfies this equation, we determine that the leading \( p \) bits of \( x \) are zeros, and the next bit is a 1 (i.e., \( x_j = 0, n - 1 - p < j \leq n - 1, x_{n-p-1} = 1 \)). The index of the remaining substring can be determined from Eq. (4), and thus all the bits of \( x \) may be calculated recursively.
C. Deriving the final program

Now we will transform our procedure into reversible code. As the last section makes clear, a necessary step for doing this will be to code the inverse of the Schumacher function. In the spirit of FIRST_TRY, we will not worry at first about the final state of the work registers as prescribed in Eq. (18); we will initially just try to code correctly the inverse function itself. We will find that reversibility will, in this case, fall out naturally from a simple modification of our first-cut program.

**Program TRY_INVERSE**

quantum registers:

- $X$: $n$-bit register (initialized to 0)
- $Y$: $n$-bit signed arithmetic register (finalized to 0)
- $S$: $\lceil \log n \rceil$-bit register (initialized and finalized to 0)

```plaintext
for m = 0 to n do
    Y ← Y − \binom{n}{m}
    if Y ≥ 0 then S ← S + 1
for m = 0 to n do
    if S ≥ m then Y ← Y + \binom{n}{m}
for p = 0 to n − 1 do
    for i = 0 to n − p do
        if S = i and Y ≥ \binom{n−p−1}{i} then $X_{n−p−1}$ ← $X_{n−p−1}$ ⊕ 1
        if S = i and $X_{n−p−1} = 1$ then Y ← Y − \binom{n−p−1}{i}
        if $X_{n−p−1} = 1$ then S ← S − 1
```

In this code, the $m$-loop does the job of finding the $m$ for which Eq. (21) is satisfied, and putting the result in the quantum register $S$. As a byproduct of this work, it subtracts away the first term of Eq. (12) from $y$, leaving in $Y$ the value of the index $I[x,n,m]$. Actually, the $m$-loop continues to subtract binomial coefficients from $Y$ after it is supposed to; this is why $Y$ is indicated to be a “signed” register, which can be handled by doing ordinary arithmetic in a register with one extra bit (see [12]). This approach has the benefit that testing that $Y$ is non-negative only requires the examination of one bit — see the first part of Sec. [IV]. We might be tempted to avoid negative numbers by terminating the loop at the
right moment, viz:

\[
\text{for } m = 0 \text{ to } n \text{ do }
  \quad \text{if } Y < \binom{n}{m} \text{ then exit for-loop}
\]

But such an exit for-loop statement is not reversible. There appears to be no alternative to letting the first loop go to its maximum possible upper limit, which is \(n\), and then repairing the damage done by adding back the correct binomial coefficients in the second loop. Finally, at the end of the second loop, \(Y\) has the desired value of \(I[x, n, m]\), and \(S\) has the value of \(m\).

Then the third (\(p\)) loop of \textsc{Try\_Inverse} does the iterative decomposition of the index \(I[x, n, m]\). For every possible value of the leading number of zeros \(p\) (recall Eq. (7)), \textsc{Try\_Inverse} checks to see if the inequality Eq. (23) is satisfied; if it is, then the program negates one bit of the \(X\) register. Then the second if statement decrements \(Y\) by the combinatorial coefficient in Eq. (9), so that it always contains the index of the next substring. The process continues until the index is reduced to zero. Also, \(S\) is decremented so that it always contains the current value of the number of 1’s in the substring of Eq. (8). Note that, as in \textsc{First\_Try}, an inner loop (indexed by \(i\)) is introduced to avoid the need for reversible calculation of binomial coefficients like \(\binom{n-p-1}{s}\).

We now evaluate what state \textsc{Try\_Inverse} has left the registers \(Y\) and \(S\) in. In fact, a very desirable thing has “accidentally” occurred! We find that, on input state

\[
|X, Y, S\rangle = |0, y, 0\rangle,
\]

\textsc{Try\_Inverse} produces the final state

\[
|X, Y, S\rangle = |f^{-1}(y), 0, 0\rangle.
\]

Thus, with a final transposing of the \(X\) and \(Y\) registers, we obtain a program that implements the inverse of Eq. (16), so the calculation has been successfully done in-place, with the registers \(Y\) and \(S\) remaining in their initial state, having served only as “catalysts” for the calculation.
In fact, we can do even better; by a small modification of \texttt{TRY\_INVERSE}, the \(Y\) register can be eliminated entirely. This can be done by noting that, during the course of an execution of \texttt{TRY\_INVERSE}, the decrementing of \(Y\) sets each of its high-order bits to zero in succession, and, at the same time, the values of \(X\) are built up starting with the high-order bits and working down. Thus, the high-order bits of \(Y\) can be re-used to hold the results of the final calculation. It can be shown that these high-order bits are always cleared out soon enough that they can be used for the final answer; this is done by showing that in \texttt{TRY\_INVERSE}, the same bits of \(X\) and \(Y\) are never simultaneously 1. Thus, with one small modification, \texttt{TRY\_INVERSE} can be turned into our final program for the inverse of the Schumacher coding function:

**Program FINAL\_SCHUMACHER\_INVERSE**

quantum registers:
\(X\) : \(n\)-bit signed arithmetic register
\(S\) : \(\lceil\log n\rceil\)-bit arithmetic register (initialized and finalized to 0)

\[
\text{for } m = 0 \text{ to } n \text{ do } \\
\quad \text{ } X \leftarrow X - \binom{n}{m} \\
\quad \text{if } X \geq 0 \text{ then } S \leftarrow S + 1 \\
\text{for } m = 0 \text{ to } n \text{ do } \\
\quad \text{if } S \geq m \text{ then } X \leftarrow X + \binom{n}{m} \\
\text{for } p = 0 \text{ to } n - 1 \text{ do } \\
\text{for } i = 0 \text{ to } n - p \text{ do } \\
\quad \text{if } S = i \text{ and } \text{TRUNC}_{n-p-1}(X) \geq \binom{n-p-1}{i} \text{ then } X_{n-p-1} \leftarrow X_{n-p-1} \oplus 1 \\
\quad \text{if } S = i \text{ and } X_{n-p-1} = 1 \text{ then } X \leftarrow X - \binom{n-p-1}{i} \\
\quad \text{if } X_{n-p-1} = 1 \text{ then } S \leftarrow S - 1
\]

The only substantial item which has been added here is the function \texttt{TRUNC}_{j}. Invocation of \texttt{TRUNC}_{j}(X) simply says that only the \(j\) least significant bits of the quantum register \(X\) (i.e., bit 0 to bit \(j - 1\)) should be taken account of in the “\(\geq\)” comparison. This is necessary because the high-order bits are being used to store the final answer. In the final pass through the \(p\) loop, the occurrence of the zero index in \texttt{TRUNC}_{0}(X) indicates that the comparison should not be performed at all.

For completeness, we now record the final code for the Schumacher coding function itself.
Since **FINAL_SCHUMACHER_INVERSE** is done “in-place”, the direct function is literally just the time-reverse:

Program **FINAL_SCHUMACHER**

quantum registers:

- $X$: $n$-bit signed arithmetic register
- $S$: $\lceil \log n \rceil$-bit arithmetic register (initialized and finalized to 0)

for $p = n - 1$ down to 0 do

  if $X_{n-p-1} = 1$ then $S \leftarrow S + 1$

  for $i = n - p$ down to 0 do

    if $S = i$ and $X_{n-p-1} = 1$ then $X \leftarrow X + {n-p-1 \choose i}$

    if $S = i$ and $\text{TRUNC}_{n-p-1}(X) \geq {n-p-1 \choose i}$ then $X_{n-p-1} \leftarrow X_{n-p-1} \oplus 1$

for $m = n$ down to 0 do

  if $S \geq m$ then $X \leftarrow X - {n \choose m}$

for $m = n$ down to 0 do

  if $X \geq 0$ then $S \leftarrow S - 1$

  $X \leftarrow X + {n \choose m}$

**IV. Bit-Level Quantum Program for Schumacher Coding**

In this section, we explain how the statements in programs **FINAL_SCHUMACHER** and **FINAL_SCHUMACHER_INVERSE** can be implemented by a gate-array with fundamental bit-level operations. These fundamental operations are essentially Toffoli gates [16]. The Toffoli gate that negates bit $B$ iff bits $C$ and $D$ are both 1 (and doesn’t change the values of $C$ and $D$) is denoted as

$$B \leftarrow B \oplus (C \land D).$$

In [10] it is shown that such an operation can be simulated in terms of eight one-bit operations and eight XOR operations (which are of the form $B \leftarrow B \oplus C$). For convenience, we expand our repertoire of allowable basic operations to include

- $B \leftarrow B \oplus 1$
- $B \leftarrow B \oplus C$
- $B \leftarrow B \oplus \overline{C}$
- $B \leftarrow B \oplus (\overline{C} \land D)$
- $B \leftarrow B \oplus (\overline{C} \land D)$
\[ B \leftarrow B \oplus (C \lor D). \]

As with Toffoli gates, each of these gates can be simulated by at most eight one-bit operations and eight XOR operations. In many cases a quantum phase freedom can be used to simulate these in fewer one- and two-bit gates (see Appendix B).

The first step to converting the programs into gate-arrays is to “unravel” the for loops. Since the ranges of these loops are all fixed prior to any computation, this is straightforward. Next, we note that (once the for loops have been unravelled) there are essentially five types of program statements:

1. \( X \leftarrow X + k \)

2. \( \text{if } B \text{ then } X \leftarrow X + k \)

3. \( \text{if } Y > l \text{ then } X \leftarrow X + k \)

4. \( \text{if } Y = l \text{ and } B \text{ then } X \leftarrow X + k \)

5. \( \text{if } Y = l \text{ and } Z > k \text{ then } B \leftarrow B \oplus 1 \)

(where \( B \) is a bit, \( X, Y, Z \) are signed arithmetic registers, and \( k, l \) are signed integers).

Also, there are a priori upper bounds on the ranges of the arithmetic registers (and thus on the number of bits required to specify them). An arithmetic register whose range of values is known to be an integer within \([0, 2^n]\) can be naturally represented by \( n \) bits and arithmetic operations on it can be simulated by reversibly performing them modulo \( 2^n \). Also, a signed arithmetic register whose range of values is known to lie within \([-2^n, +2^n]\) can be naturally represented in “two’s complement” form by \( n + 1 \) bits, and it is well known that arithmetic operations on such a two’s complement integer can be simulated by interpreting it as an integer in the range \([0, 2^{n+1}]\) and performing arithmetic modulo \( 2^{n+1} \) (see, for example, [17]).

**A. Addition and Conditional Addition**

In view of the above discussion, to simulate
if $B$ then $X \leftarrow X + k$,

it suffices to perform

$$X \leftarrow (X + B \cdot k) \mod 2^n$$

(in other words to add $k$ to $X$ modulo $2^n$ iff $B = 1$). In the case where $X$ is an $n$-bit signed register, it suffices to substitute $n + 1$ for $n$ above.

The program below performs this using $n$ auxiliary bits $C_0, C_1, \ldots, C_{n-1}$ (which are assumed to have initial value 0, and are reset to 0 by the end of the computation).

**Program CONDITIONAL_ADD**

quantum registers:

- $X$: $n$-bit signed arithmetic register
- $B$: bit register
- $C_0, C_1, \ldots, C_{n-1}$: bit registers (initialized and finalized to 0)

for $i = 1$ to $n - 1$

$$C_i \leftarrow C_i \oplus \text{MAJ}(k_{i-1}, X_{i-1}, C_{i-1})$$

for $i = n - 1$ down to 1

$$X_i \leftarrow X_i \oplus (k_i \wedge B)$$
$$X_i \leftarrow X_i \oplus (C_i \wedge B)$$
$$C_i \leftarrow R C_i \oplus \text{MAJ}(k_{i-1}, X_{i-1}, C_{i-1})$$

$X_0 \leftarrow X_0 \oplus k_0$

where

$$\text{MAJ}(l, S, T) = \begin{cases} S \wedge T & \text{if } l = 0 \\ S \lor T & \text{if } l = 1. \end{cases}$$

The number of basic operations performed by the above program is bounded above by $4n + O(1)$. In particular, if the for loops of this program are unravelled then the program corresponds to a gate-array consisting of $2n + 1$ bits and $4n + O(1)$ gates. (A more space-efficient $(n + O(\sqrt{n}))$-bit program is described in Appendix A.)

The unconditional addition statement

$$X \leftarrow X + k$$

can be easily simulated by replacing $(k_i \wedge B)$ and $(C_i \wedge B)$ in the above program with $k_i$ and $C_i$ (respectively).

**CONDITIONAL_ADD** introduces two modified assignment symbols “$\leftarrow \subset$” and
For the present purposes these can be thought of as identical to the ordinary “←” assignment; however, they signal a freedom in how the quantum phase may be handled in these assignments, as discussed in Appendix B.

One final note about **CONDITIONAL_ADD**: it involves only the addition of a quantum register with an ordinary, classical number. It is possible to write a similar program which adds two quantum registers, as has been illustrated in [12]; however, this more complex routine is never needed for the implementation of the Schumacher function. Actually, it is generally possible to implement a full quantum adder as a sequence of calls to **CONDITIONAL_ADD**.

### B. Equality and Inequality Testing

In order to simulate the remaining types of statements, it suffices to simulate *equality test* statements of the form

\[ B \leftarrow B \oplus (X = k) \]

(which negate \( B \) iff \( X = k \)), and *inequality test* statements of the form

\[ B \leftarrow B \oplus (X > k) \]

(which negate \( B \) iff \( X > k \)).

With implementations of the above tests, the statement

\[ \text{if } Y > l \text{ then } X \leftarrow X + k \]

is then easily simulated by the sequence

\[ B \leftarrow B \oplus (Y > l) \]
\[ \text{if } B \text{ then } X \leftarrow X + k \]
\[ B \leftarrow B \oplus (Y > l) \]

where \( B \) is a bit register distinct from the bits of \( X \) and \( Y \), and whose initial value is 0 (note that \( B \) must be reset to 0 after the addition is performed). Also, the compound conditional

\[ \text{if } Y = l \text{ and } B \text{ then } X \leftarrow X + k \]

is simulated by the sequence

\[ B \leftarrow B \oplus (Y = l) \]
\[ \text{if } B \text{ then } X \leftarrow X + k \]
\[ B \leftarrow B \oplus (Y = l) \]
\[ C \leftarrow C \oplus (Y = l) \]
\[ D \leftarrow D \oplus (C \wedge B) \]
\[ \text{if } D \text{ then } X \leftarrow X + k \]
\[ D \leftarrow_R D \oplus (C \wedge B) \]
\[ C \leftarrow_R C \oplus (Y = l) \]

where \( C \) and \( D \) are bit registers distinct from the bits of \( X, Y, \) and \( B, \) and whose initial (and final) values are 0. Again, the meaning and usefulness of the phase-modified assignments is discussed in Appendix B.

The following program simulates an equality test. It uses \( n \) auxiliary bit registers \( C_0, C_1, \ldots, C_{n-1}. \) The auxiliary registers are initialized to 0, and have final value 0.

Program TEST_EQUALITY_TO_k

quantum registers:
\( X \) : \( n \)-bit signed arithmetic register
\( B \) : bit register
\( C_0, C_1, \ldots, C_{n-1} \) : bit registers (initialized and finalized to 0)

\[ C_{n-1} \leftarrow C_{n-1} \oplus (X_{n-1} = k_{n-1}) \]
for \( i = n - 2 \) down to 0 do
\[ C_i \leftarrow C_i \oplus (C_{i+1} \wedge (X_i = k_i)) \]
\[ B \leftarrow B \oplus C_0 \]
for \( i = 0 \) to \( n - 2 \) do
\[ C_i \leftarrow_R C_i \oplus (C_{i+1} \wedge (X_i = k_i)) \]
\[ C_{n-1} \leftarrow_R C_{n-1} \oplus (X_{n-1} = k_{n-1}) \]

where
\[
(S = l) = \begin{cases} 
\overline{S} & \text{if } l = 0 \\
S & \text{if } l = 1.
\end{cases}
\]

The number of basic operations performed by the above program is bounded above by \( 2n + O(1) \). (The above program is very similar to the so-called \( \wedge_n \)-gate construction in [10]).

Finally, the following program simulates an inequality test. It uses \( n \) auxiliary bit registers \( C_0, C_1, \ldots, C_{n-1}. \) The auxiliary registers are initialized to 0, and have final value 0.

Program TEST_GREATER_THAN_k
quantum registers:
X: n-bit signed arithmetic register
B: bit register
C_0, C_1, . . . , C_{n-1}: bit registers (initialized and finalized to 0)

C_{n-1} \leftarrow C_{n-1} \oplus (X_{n-1} = k_{n-1})
B \leftarrow B \oplus (X_{n-1} < k_{n-1})
for \ i = n - 2 \text{ down to } 0 \ do
\quad C_i \leftarrow C_i \oplus (C_{i+1} \land (X_i = k_i))
\quad B \leftarrow B \oplus C_{i+1} \land (X_i > k_i)
for \ i = 0 \text{ down to } n - 2 \ do
\quad C_i \leftarrow_R C_i \oplus (C_{i+1} \land (X_i = k_i))
\quad C_{n-1} \leftarrow_R C_{n-1} \oplus (X_{n-1} = k_{n-1})

where \ ((S = l)) \ is \ as \ in \ the \ previous \ subsection,
\( (S > l) = \begin{cases} 
S & \text{if } l = 0 \\
0 & \text{if } l = 1,
\end{cases} \)

and
\( (S < l) = \begin{cases} 
0 & \text{if } l = 0 \\
S & \text{if } l = 1.
\end{cases} \)

The number of basic operations performed by the above program is bounded above by
3n + O(1). Once again, we employ phase-modified assignments \( \leftarrow \), \( \leftarrow_R \), and \( \leftarrow \) which are
explained in Appendix B.

V. DISCUSSION AND CONCLUSIONS

We can finally put all the above results together to evaluate the total cost, in time and
space, to perform Schumacher coding. It is easy to see that the two if statements inside the
i loop of FINAL SCHUMACHER are the most expensive part of the procedure. The
first if statement requires one call to CONDITIONAL ADD. Although X is an n-bit
register, the addition only affects the \( n - p - 1 \) low-order bits of X. Thus, the addition can
be performed on TRUNC_{n-p-1}(X) rather than X, which amounts to a total running time of
\[
\sum_{p=0}^{n-1} \sum_{i=0}^{n-p} 4(n - p - 1) + O(1) = \frac{2}{3}n^3 + O(n^2). \tag{26}
\]

The expensive part of the second if statement is its two calls to \texttt{TEST\_GREATER\_THAN}, performed on an \((n - p - 1)\)-bit quantum register (because of the action of \texttt{TRUNC}). The time involved for this is

\[
\sum_{p=0}^{n-1} \sum_{i=0}^{n-p} 2 \cdot 3(n - p - 1) + O(1) = n^3 + O(n^2). \tag{27}
\]

Thus, the total time required (i.e., number of bit-level primitive steps) is \(\frac{2}{3}n^3 + O(n^2)\). The total number qubits used is: \(n\), to hold the input/output string \(X\); plus \(\lceil \log n \rceil\), to hold \(S\); plus \(n + O(1)\) to implement the conditional additions and inequality tests (the same work registers that store carries and so forth may be reused throughout the execution of the program). Thus, the total number of qubits is \(2n + \lceil \log n \rceil + O(1)\).

If the space-efficient routines \texttt{CONDITIONAL\_ADD'} and \texttt{TEST\_GREATER\_THAN'} introduced in Appendix A are used instead, the execution time is increased to \(\frac{8}{3}n^3 + O(n^{2.5})\), but the total number of qubits is reduced to \(n + 2\sqrt{n} + O(\log n)\). If the relevant figure of merit for the tractability of the quantum computation is the product of time and space, as it is in certain physical models [7,8], then the space-efficient procedures we have introduced would be preferred.

A final note about these operation counts: they are all in terms of the primitive operations listed at the beginning of Section IV, which includes both two- and three-bit primitives. It is known [10,18] that all three-bit operations can be simulated in quantum logic by a sequence of two-bit primitives. Most of the three-bit operations can be simulated using seven operations (3 quantum XORs and 4 one-bit gates); see Appendix B. So, in terms of these primitive operations the total time to do the Schumacher function would be roughly \(7 \cdot \frac{2}{3}n^3 < 19n^3\). Computing the exact prefactor would require a considerable amount of detailed calculation, and would have to take into account that fact that many one-bit gates in the network could be merged together and executed in one step (see [10]). All of this work could easily be done if an actual physical implementation of Schumacher compression were ever undertaken.
To conclude, we believe that the pseudocode in which our results are presented is the most concise and economical form in which to present a quantum computation like Schumacher coding. The bit level primitives for addition and comparison which we have presented are similar to ones which have been presented elsewhere [12], but have a few features which may make them superior in the development of other quantum programs. The Schumacher coding can be done in $O(n^3)$ steps, with $O(\sqrt{n})$ auxiliary workspace. We cannot exclude the possibility that a lower polynomial-order algorithm may be found, but we are not presently aware of what form this would take. The techniques in [14] enable further shrinkage of the auxiliary workspace, but with a larger penalty in the running time. We think that further useful shrinkage of the auxiliary workspace is unlikely; in the present scheme, only a vanishingly small fraction of quantum bits are used as workspace for large blocksize $n$.

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APPENDIX A: IMPROVEMENTS IN THE WORKSPACE EFFICIENCY OF THE BIT-LEVEL IMPLEMENTATIONS

The bit-level implementations proposed in Sections IV A and IV B require $n$ auxiliary bit registers. By applying techniques that were introduced in [14], we derive the following alternate programs that employ only $O(\sqrt{n})$ auxiliary bit registers while maintaining the same asymptotic operation complexity. (The space-reduction techniques in [14], can also be used to reduce the auxiliary space further, but this incurs an increase in the running time, as well as in the space-time product.)

Assume that $n = m^2$. The program `CONDITIONAL_ADD′\textsubscript{$k$}` that follows employs $2m - 1$ auxiliary bit registers rather than the $n$ auxiliary bit registers that CONDI-
**TIONAL_ADD** \(_k\) employs. In **CONDITIONAL_ADD** \(_k\), registers \(C_0, \ldots, C_{n-1}\) are used to store information about carry propagation. In **CONDITIONAL_ADD** \(_k\), this is accomplished by registers \(C_1, \ldots, C_{m-1}\) and \(D_1, \ldots, D_{m-1}\) instead. The idea is to reset some of the registers to 0 at various checkpoints during the course of the computation. This is illustrated by the diagram below, where the horizontal direction represents time, and the placement of the lines indicate the time intervals during which the registers are active, containing the various carry bits. Registers \(D_1, \ldots, D_{m-1}, C_1\) are first set to the first \(m\) carry bits. Then \(D_1, \ldots, D_{m-1}\) are reset to 0. Registers \(D_1, \ldots, D_{m-1}, C_2\) can then be used to store the \(m + 1^{\text{st}}\) to \(2m^{\text{th}}\) carry bits and then \(D_1, \ldots, D_{m-1}\) are reset to 0 again — since \(C_1\) stores the \(m^{\text{th}}\) carry bit, this can be accomplished without recomputing the first \(m\) carry bits. The process is repeated with the remaining carry bits, and then applied in reverse to reset the carry bits to 0, as illustrated here:

| carry bits | registers used |
|------------|----------------|
| \(m^2 - 1\) | \(D_{m-1}\) |
| \((m - 1)m + 2\) | \(D_2\) |
| \((m - 1)m + 1\) | \(D_1\) |
| \((m - 1)m\) | \(C_{m-1}\) |
| \(3m\) | \(C_3\) |
| \(3m - 1\) | \(D_{m-1}\) |
| \(2m + 2\) | \(D_2\) |
| \(2m + 1\) | \(D_1\) |
| \(2m\) | \(C_2\) |
| \(2m - 1\) | \(D_{m-1}\) |
| \(m + 2\) | \(D_2\) |
| \(m + 1\) | \(D_1\) |
| \(m\) | \(C_1\) |
| \(m - D_{m-1}\) | \(D_2\) |
| 2 | \(D_1\) |
| 1 | \(D_0\) |

The detailed program follows. \(D_0\) is used for convenience to store the value of \(C_i\) at the beginning of each iteration of the for-loop with respect to \(i\).
Program CONDITIONAL_ADD′\$k$

quantum registers:
\( X \) : \( n \)-bit arithmetic register
\( B \) : bit register
\( C_1, C_2, \ldots, C_{m-1} \) : bit registers (initialized and finalized to 0)
\( D_0, D_1, \ldots, D_{m-1} \) : bit registers (initialized and finalized to 0)

for \( i = 0 \) to \( m - 2 \) do
  if \( i > 0 \) then \( D_0 \leftarrow D_0 \oplus C_i \)
  for \( j = 1 \) to \( m - 1 \) do
    \( D_j \leftarrow D_j \oplus \text{MAJ}(k_{im+j-1}, X_{im+j-1}, D_{j-1}) \)
    \( C_{i+1} \leftarrow C_{i+1} \oplus \text{MAJ}(k_{im+m-1}, X_{im+m-1}, D_{m-1}) \)
  for \( j = m - 1 \) down to 1 do
    \( D_j \leftarrow R D_j \oplus \text{MAJ}(k_{im+j-1}, X_{im+j-1}, D_{j-1}) \)
  if \( i > 0 \) then \( D_0 \leftarrow D_0 \oplus C_i \)

\( D_0 \leftarrow D_0 \oplus C_{m-1} \)

for \( j = 1 \) to \( m - 1 \) do
  \( D_j \leftarrow D_j \oplus \text{MAJ}(k_{(m-1)m+j-1}, X_{(m-1)m+j-1}, D_{j-1}) \)
for \( j = m - 1 \) down to 1 do
  \( X_{(m-1)m+j} \leftarrow X_{(m-1)m+j} \oplus (k_{(m-1)m+j} \land B) \)
  \( X_{(m-1)m+j} \leftarrow X_{(m-1)m+j} \oplus (D_j \land B) \)
  \( D_j \leftarrow R D_j \oplus \text{MAJ}(k_{(m-1)m+j-1}, X_{(m-1)m+j-1}, D_{j-1}) \)
\( D_0 \leftarrow D_0 \oplus C_{m-1} \)

for \( i = m - 2 \) down to 0 do
  if \( i > 0 \) then \( D_0 \leftarrow D_0 \oplus C_i \)
  for \( j = 1 \) to \( m - 1 \) do
    \( D_j \leftarrow D_j \oplus \text{MAJ}(k_{im+j-1}, X_{im+j-1}, D_{j-1}) \)
    \( X_{im+m} \leftarrow X_{im+m} \oplus (k_{im+m} \land B) \)
    \( X_{im+m} \leftarrow X_{im+m} \oplus (C_{i+1} \land B) \)
    \( C_{i+1} \leftarrow R C_{i+1} \oplus \text{MAJ}(k_{im+m-1}, X_{im+m-1}, D_{m-1}) \)
  for \( j = m - 1 \) down to 1 do
    \( X_{im+j} \leftarrow X_{im+j} \oplus (k_{im+j} \land B) \)
    \( X_{im+j} \leftarrow X_{im+j} \oplus (D_j \land B) \)
    \( D_j \leftarrow R D_j \oplus \text{MAJ}(k_{im+j-1}, X_{im+j-1}, D_{j-1}) \)
  if \( i > 0 \) then \( D_0 \leftarrow D_0 \oplus C_i \)

\( X_0 \leftarrow X_0 \oplus k_0 \)
The above program uses \( n + O(\sqrt{n}) \) registers in total and runs in \( 6n + O(\sqrt{n}) \) steps (compared to \( 2n + O(\log n) \) registers in total and \( 4n + O(1) \) steps for \texttt{CONDITIONAL\_ADD\_k}.

There also exist more space-efficient versions of \texttt{TEST\_EQUALITY\_TO\_k} and \texttt{TEST\_GREATER\_THAN\_k}. For the former case, the program is as follows (where again \( n = m^2 \)).

**Program \texttt{TEST\_EQUALITY\_TO\_k}**

quantum registers:
- \( X \) : \( n \)-bit arithmetic register
- \( B \) : bit register
- \( C_0, C_1, \ldots, C_{m-1} \) : bit registers (initialized and finalized to 0)
- \( D_1, D_2, \ldots, D_m \) : bit registers (initialized and finalized to 0)

for \( i = m - 1 \) down to 0 do
  if \( i = m - 1 \) then \( D_m \leftarrow D_m \oplus 1 \) else \( D_m \leftarrow D_m \oplus C_{i+1} \)
  for \( j = m - 1 \) down to 1 do
    \( D_j \leftarrow D_j \oplus (D_{j+1} \land (X_{im+j} = k_{im+j})) \)
    \( C_i \leftarrow C_i \oplus (D_1 \land (X_{im} = k_{im})) \)
  for \( j = 1 \) to \( m - 1 \) do
    \( D_j \leftarrow R D_j \oplus (D_{j+1} \land (X_{im+j} = k_{im+j})) \)
  if \( i = m - 1 \) then \( D_m \leftarrow D_m \oplus 1 \) else \( D_m \leftarrow D_m \oplus C_{i+1} \)

\( B \leftarrow B \oplus C_0 \)

for \( i = 0 \) to \( m - 1 \) do
  if \( i = m - 1 \) then \( D_m \leftarrow D_m \oplus 1 \) else \( D_m \leftarrow D_m \oplus C_{i+1} \)
  for \( j = m - 1 \) down to 1 do
    \( D_j \leftarrow D_j \oplus (D_{j+1} \land (X_{im+j} = k_{im+j})) \)
    \( C_i \leftarrow R C_i \oplus (D_1 \land (X_{im} = k_{im})) \)
  for \( j = 1 \) to \( m - 1 \) do
    \( D_j \leftarrow R D_j \oplus (D_{j+1} \land (X_{im+j} = k_{im+j})) \)
  if \( i = m - 1 \) then \( D_m \leftarrow D_m \oplus 1 \) else \( D_m \leftarrow D_m \oplus C_{i+1} \)

The above program uses \( n + O(\sqrt{n}) \) registers in total and runs in \( 4n + O(\sqrt{n}) \) steps (compared to \( 2n + O(1) \) registers in total and \( 2n + O(1) \) steps for \texttt{TEST\_EQUALITY\_TO\_k}.

The program \texttt{TEST\_GREATER\_THAN\_k} is similar to the above attaining \( 5n + \)}
$O(\sqrt{n})$ time and $n + O(\sqrt{n})$ space (vs. $3n + O(1)$ time and $2n + O(1)$ space).

**APPENDIX B: PHASE FREEDOM IN IMPLEMENTATION OF REVERSIBLE ROUTINES**

Here we will explain ways in which the quantum phase can be treated in the essentially classical reversible routines which we have been discussing throughout this paper. In the language of quantum logic gates, the bit-level logic statements used in the programs here are represented by unitary matrices applied to the quantum wavefunction of all the registers. These unitary matrices have a special restriction which make them “classical”, which is that the matrix elements are only zero or one; this means that every definite computational state $|x\rangle$ is taken to another definite computational state $|f(x)\rangle$, and not to a superposition of states. To give an example, the Toffoli gate, the three-bit implementation of the AND gate in reversible logic, involves the following unitary matrix:

\[
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}.
\] (B1)

Here we consider the question of whether elementary operations with modified phases (i.e., in which the matrix elements are unimodular complex numbers $e^{i\theta}$, rather than being 1) could be used in the implementation of the Schumacher function. We are motivated to investigate this because we found in our previous study [10] that the implementation of a modified Toffoli gate with a single non-zero phase
requires fewer resources in the following sense: we showed that the zero-phase Toffoli gate (Eq. (B1)) can be implemented with 8 two-bit XOR gates and 8 one-bit gates, while the Toffoli gate with modified phases (Eq. (B2)) requires only 3 XOR’s and 4 one-bit gates. We will establish here that the less-costly gate can in fact be used for most of the Toffoli gates, and related three-bit operations, that are used in the implementation of the Schumacher compression function.

Note that it is necessary that the complete Schumacher calculation be carried out with all the quantum phases equal to zero, in order that the superposition states discussed in Section I maintain the correct phase relation to one another. Thus the question becomes: how can the effect of the non-zero phase in Eq. (B2), if it is introduced in one Toffoli gate, be undone at some later step of the calculation? The answer (which we will establish shortly) is the obvious one: many of the reversible routines which we have introduced (although not the high-level Schumacher program itself) have a palindromic character, so that a Toffoli gate on three bits is exactly “undone” at a later stage of the computation, roughly as far from the end of the subroutine as the original gate is from the beginning. It turns out that the effect of the \(-1\) phase factor can be precisely undone at the second occurrence of the gate, too.
We will now establish the desired basic result using the setup of the figure, that the boolean function $f$ can be implemented with any arbitrary phase factors, so long as they also appear in $f^{-1}$, no matter what the intervening boolean function $g$ is, so long as $g$ does not modify the values of the bits on which $f$ and $f^{-1}$ act. By applying this result repeatedly to the subroutines which we have introduced, starting at the innermost level, we deduce all the three-bit primitives which can be implemented with non-zero phase. Assignments in which these non-zero phases are permitted have been identified by the special assignment symbol

$$\leftarrow \subset.$$  \hspace{1cm} (B3)

These statements are always paired with others, denoted by

$$\leftarrow \in R,$$ \hspace{1cm} (B4)

in which the reverse phases are implemented. (For the phases in Eq. (B2), the operation is self-inverse.) In one case, the pairing is between statements in different, palindromically-arranged calls of the same subroutine; for these we have used a distinct symbol

$$\leftarrow <.$$ \hspace{1cm} (B5)
After establishing the basic result, we will review a few of the details of this implementation in the Schumacher function.

Let us first write down what the set of operations in the figure is supposed to do. Beginning with the basis state

$$|x⟩ = |x_1x_2...x_n...x_m⟩$$ (B6)

at time $t_1$, it becomes at $t_2$, after the operation of $f$,

$$|x'⟩ = |f(x_1x_2...x_n)x_{n+1}...x_m⟩$$ (B7)

Then at time $t_3$ the state is

$$\exp(iθg(x'))|f(x_1x_2...x_n)g(x')⟩.$$ (B8)

$g(x')$ depends on the state of the entire $m$-bit register $x'$, but only modifies the last $m-n$ bits, as indicated. Note that we allow for the possibility that $g$ itself is a modified boolean function with non-zero phases. This is necessary because we will apply this result in a nested fashion in the Schumacher subroutines. Finally at time $t_4$ the state is

$$\exp(iθg(x))|x_1x_2...x_ng(x')⟩.$$ (B9)

That is, the first $n$ bits are restored to their original state, and bits $n+1$ through $m$ remain in the state $g(x)$.

Now, the question is, will the state Eq. (B9) still result if the function $f$ is modified to introduce non-zero phases $θf(x_1...x_n)$? If we establish that this is true for all boolean inputs $|x⟩$, this will suffice to prove that these networks have the same action on any arbitrary quantum states (this follows directly from the linear superposition principle of quantum mechanics). We follow the time evolution as before with the modified $f$. At time $t_2$ the state is

$$\exp(iθf(x_1...x_n))|f(x_1x_2...x_n)x_{n+1}...x_m⟩$$ (B10)
Then at time $t_3$:

$$\exp(i(\theta_g(x') + \theta_f(x_1...x_n))) | f(x_1x_2...x_n)g(x') \rangle$$  \hspace{1cm} (B11)

and finally at $t_4$:

$$\exp(i(\theta_f(x_1...x_n) + \theta_g(x') + \theta_{f^{-1}}(f(x_1...x_n))) | x_1x_2...x_ng(x') \rangle$$  \hspace{1cm} (B12)

The final term in the phase factor can be simplified. Recall that the unitary transformation corresponding to $f^{-1}$ is the transpose of the complex conjugate of the unitary transformation corresponding to $f$. (This follows directly from the definition of unitarity.) Therefore, to get $\theta_{f^{-1}}$ from $\theta_f$, we flip the sign (this is the complex conjugation), and we make the argument of the $\theta$ function the output values of the bits rather than the input values (this is the transpose). Here we use the fact that $g$ does not modify the first $n$ bits — their output values are the same as the original inputs $x_1x_2...x_n$. Rendering this in mathematical language:

$$\theta_{f^{-1}}(f(x_1...x_n)) = -\theta_f(x_1...x_n)$$  \hspace{1cm} (B13)

Thus, the two $\theta_f$ terms in the phase in Eq. (B12) cancel out, and Eq. (B12) becomes identical to Eq. (B9), which is the desired result. \Box

Finally, we briefly review the application of this result to the programs introduced in the text. The first appearance is in \texttt{CONDITIONAL ADD \_k}, where the role of $f$ is played in the innermost part of the program by the assignment statement

$$C_{n-1} \leftarrow C_{n-1} \oplus \text{MAJ}(k_{n-2}, X_{n-2}, C_{n-2})$$

This is a three-bit operation of the Toffoli type (or a trivial modification of it) involving the bits $C_{n-1}$, $C_{n-2}$, and $X_{n-2}$. $f^{-1}$ occurs a short distance down,

$$C_{n-1} \leftarrow R C_{n-1} \oplus \text{MAJ}(k_{n-2}, X_{n-2}, C_{n-2})$$

The role of $g$ is played by the two statements
\[
X_{n-1} \leftarrow X_{n-1} \oplus (k_{n-1} \land B) \\
X_{n-1} \leftarrow X_{n-1} \oplus (C_{n-1} \land B)
\]

Obviously, only \(X_{n-1}\) is modified by \(g\), so the condition that \(g\) modify only bits not touched by \(f\) is satisfied; so, we are allowed to introduce a phase-modified \(f\) as indicated by the \(\leftarrow \) and \(\leftarrow_R\) assignments. Moving away from the innermost part of the program, we see that all the above is nested inside a larger \(g\) in which \(C_{n-1}, X_{n-2}\), and \(X_{n-1}\) are modified, surrounded by a \(f - f^{-1}\) pair involving the bits \(C_{n-2}, X_{n-3}\), and \(C_{n-3}\); working outward in succession this way, we conclude that all the \(C_i\) assignments may be replaced with phase-modified \(\leftarrow \) and \(\leftarrow_R\) assignments.

In Section IVB we exhibit a pair of statements

\[
B \leftarrow B \oplus (Y > l) \\
B \leftarrow_R B \oplus (Y > l)
\]

playing the role of \(f\) and \(f^{-1}\). These are not primitive three-bit operations as in the earlier examples, but they are themselves implemented with bit-level programs (\textsc{Test Greater Than \(k\)}). For this \(f^{-1}\), the \(\leftarrow_R\) assignment requires that the bit-level routine be run in the time-reversed order. This can be done since classically, this boolean function is its own inverse. In the time-inverted \textsc{Test Greater Than \(k\)}, the \(\leftarrow\)'s and \(\leftarrow_R\)'s should be interchanged. The \(B\) assignment involving the symbol \(\leftarrow\) in this routine is special, in that it is paired with the same statement in the time-reversed call to \textsc{Test Greater Than \(k\)}. This special symbol is a reminder is that this statement should be implemented with the phases corresponding to the \(\leftarrow\) assignment in the first call to the program, and with those corresponding to the \(\leftarrow_R\) assignment in the second call.

We have not indicated phase-modifying assignments for any of the two-bit gate level operations in these programs. We take as given that these two-bit gates could be implemented with zero phases. But if this were not the case, then many of these paired assignments may be phase-modified in exactly the way we have shown for the three-bit primitives.
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