Figure III.9: Left: classical gates. Right: controlled-NoT gate. [from Nielsen & Chuang (2010, Fig. 1.6)]

C.2 Quantum gates

Quantum gates are analogous to ordinary logic gates (the fundamental building blocks of circuits), but they must be unitary transformations (see Fig. III.9, left, for ordinarty logic gates). Fortunately, Bennett, Fredkin, and Toffoli have already shown how all the usual logic operations can be done reversibly. In this section you will learn the most important quantum gates.

C.2.a SINGLE-QUBIT GATES

The NOT gate is simple because it is reversible: $NOT|0\rangle = |1\rangle$, $NOT|1\rangle = |0\rangle$. Its desired behavior can be represented:

$$\begin{array}{cccc} \mathrm{NOT}: & & |0\rangle & \mapsto & |1\rangle \\ & & |1\rangle & \mapsto & |0\rangle. \end{array}$$

Note that defining it on a basis defines it on all quantum states. Therefore it can be written as a sum of dyads (outer products):

$$NOT = |1\rangle\langle 0| + |0\rangle\langle 1|.$$

You can read this, "return $|1\rangle$ if the input is $|0\rangle$, and return $|0\rangle$ if the input is $|1\rangle$." Recall that in the standard basis $|0\rangle = (1 \ 0)^{T}$ and $|1\rangle = (0 \ 1)^{T}$.

Therefore NOT can be represented in the standard basis by computing the outer products:

$$NOT = \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 \ 0) + \begin{pmatrix} 1 \\ 0 \end{pmatrix} (0 \ 1) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The first column represents the result for $|0\rangle$, which is $|1\rangle$, and the second represents the result for $|1\rangle$, which is $|0\rangle$.

Although NOT is defined in terms of the computational basis vectors, it applies to any qubit, in particular to superpositions of $|0\rangle$ and $|1\rangle$:

$$NOT(a|0\rangle + b|1\rangle) = aNOT|0\rangle + bNOT|1\rangle = a|1\rangle + b|0\rangle = b|0\rangle + a|1\rangle.$$

Therefore, NOT exchanges the amplitudes of $|0\rangle$ and $|1\rangle$.

In quantum mechanics, the NOT transformation is usually called X. It is one of four useful unitary operations, called the *Pauli matrices*, which are worth remembering. In the standard basis:

$$I \stackrel{\text{def}}{=} \sigma_0 \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{III.10}$$

$$X \stackrel{\text{def}}{=} \sigma_x \stackrel{\text{def}}{=} \sigma_1 \stackrel{\text{def}}{=} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
 (III.11)

$$Y \stackrel{\text{def}}{=} \sigma_y \stackrel{\text{def}}{=} \sigma_2 \stackrel{\text{def}}{=} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$
 (III.12)

$$Z \stackrel{\text{def}}{=} \sigma_z \stackrel{\text{def}}{=} \sigma_3 \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
 (III.13)

We have seen that X is NOT, and I is obviously the identity gate. Z leaves $|0\rangle$ unchanged and maps $|1\rangle$ to $-|1\rangle$. It is called the phase-flip operator because it flips the phase of the $|1\rangle$ component by π relative to the $|0\rangle$ component. (Recall that global/absolute phase doesn't matter.) The Pauli matrices span the space of 2×2 complex matrices (Exer. III.18).

Note that $Z|+\rangle = |-\rangle$ and $Z|-\rangle = |+\rangle$. It is thus the analog in the sign basis of X (NOT) in the computational basis. What is the effect of Y on the computational basis vectors? (Exer. III.12)

Note that there is an alternative definition of Y that differs only in global phase:

$$Y \stackrel{\text{def}}{=} \left(\begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right).$$

This is a $90^{\circ} = \pi/2$ counterclockwise rotation: $Y(a|0\rangle + b|1\rangle) = b|0\rangle - a|1\rangle$. Draw a diagram to make sure you see this.

Note that the Pauli operations apply to any state, not just basis states. The X, Y, and Z operators get their names from the fact that they reflect state vectors along the x, y, z axes of the Bloch-sphere representation of a qubit, which we will not use in this book. Since they are reflections, they are Hermitian (their own inverses).

C.2.b Multiple-qubit gates

We know that any logic circuit can be built up from NAND gates. Can we do the same for quantum logic, that is, is there a universal quantum logic gate? We can't use NAND, because it's not reversible, but we will see that there are universal sets of quantum gates.

The *controlled-NOT* or CNOT gate has two inputs: the first determines what it does to the second (negate it or not).

CNOT:
$$|00\rangle \mapsto |00\rangle$$

 $|01\rangle \mapsto |01\rangle$
 $|10\rangle \mapsto |11\rangle$
 $|11\rangle \mapsto |10\rangle$.

Its first argument is called the *control* and its second is called the *target*, *controlled*, or *data* qubit. It is a simple example of conditional quantum computation. CNOT can be translated into a sum-of-dyads representation (Sec. A.2.d), which can be written in matrix form (Ex. III.21, p. 194):

CNOT =
$$|00\rangle\langle00|$$

+ $|01\rangle\langle01|$
+ $|11\rangle\langle10|$
+ $|10\rangle\langle11|$

We can also define it (for $x, y \in \mathbf{2}$), $\text{CNOT}|xy\rangle = |xz\rangle$, where $z = x \oplus y$, the exclusive OR of x and y. That is, $\text{CNOT}|x,y\rangle = |x,x \oplus y\rangle$ CNOT is the only non-trivial 2-qubit reversible logic gate. Note that CNOT is unitary since obviously $\text{CNOT} = \text{CNOT}^{\dagger}$ (which you can show using its dyadic representation or its matrix representation, Ex. III.21, p. 194). See the right

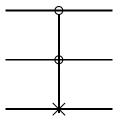


Figure III.10: Diagram for CCNOT or Toffoli gate [fig. from Nielsen & Chuang (2010)]. Sometimes the \times is replaced by \oplus because CCNOT $|xyz\rangle = |x, y, xy \oplus z\rangle$.

panel of Fig. III.9 (p. 104) for the matrix and note the diagram notation for CNOT.

CNOT can be used to produce an entangled state:

$$\operatorname{CNOT}\left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right]|0\rangle = \operatorname{CNOT}\frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = |\beta_{00}\rangle.$$

Note also that $\text{CNOT}|x,0\rangle = |x,x\rangle$, that is, FAN-OUT, which would seem to violate the No-cloning Theorem, but it works as expected only for $x \in \mathbf{2}$. In general $\text{CNOT}|\psi\rangle|0\rangle \neq |\psi\rangle|\psi\rangle$ (Exer. III.22).

Another useful gate is the three-input/output *Toffoli gate* or *controlled-controlled-NOT*. It negates the third qubit if and only if the first two qubits are both 1. For $x, y, z \in \mathbf{2}$,

$$\begin{array}{ccc} \text{CCNOT}|1,1,z\rangle & \stackrel{\text{def}}{=} & |1,1,\neg z\rangle, \\ \text{CCNOT}|x,y,z\rangle & \stackrel{\text{def}}{=} & |x,y,z\rangle, & \text{otherwise}. \end{array}$$

That is, $\text{CCNOT}|x,y,z\rangle = |x,y,xy \oplus z\rangle$. All the Boolean operations can be implemented (reversibly!) by using Toffoli gates (Exer. III.25). For example, $\text{CCNOT}|x,y,0\rangle = |x,y,x \wedge y\rangle$. Thus it is a universal gate for quantum logic. In Jan. 2009 CCNOT was implemented successfully using trapped ions.⁵

⁵Monz, T.; Kim, K.; Hänsel, W.; Riebe, M.; Villar, A. S.; Schindler, P.; Chwalla, M.; Hennrich, M. et al. (Jan 2009). "Realization of the Quantum Toffoli Gate with Trapped Ions." *Phys. Rev. Lett.* **102** (4): 040501. arXiv:0804.0082.

C.2.c Walsh-Hadamard transformation

Recall that the sign basis is defined $|+\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|-\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. The *Hadamard transformation* or *gate* is defined:

$$H|0\rangle \stackrel{\text{def}}{=} |+\rangle,$$
 (III.14)

$$H|1\rangle \stackrel{\text{def}}{=} |-\rangle.$$
 (III.15)

In sum-of-dyads form: $H \stackrel{\text{def}}{=} |+\chi 0| + |-\chi 1|$. In matrix form (with respect to the standard basis):

$$H \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix}. \tag{III.16}$$

Note that H is self-adjoint, $H^2 = I$ (since $H^{\dagger} = H$). H can be defined also in terms of the Pauli matrices: $H = (X + Z)/\sqrt{2}$ (Exer. III.33).

The H transform can be used to transform the computational basis into the sign basis and back (Exer. III.32):

$$H(a|0\rangle + b|1\rangle) = a|+\rangle + b|-\rangle,$$

 $H(a|+\rangle + b|-\rangle) = a|0\rangle + b|1\rangle.$

Alice and Bob could use this in quantum key distribution.

When applied to a $|0\rangle$, H generates an (equal-amplitude) superposition of the two bit-values, $H|0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$. This is a useful way of generating a superposition of both possible input bits, and the Walsh transform, a tensor power of H, can be applied to a quantum register to generate a superposition of all possible register values. Consider the n=2 case:

$$H^{\otimes 2}|\psi,\phi\rangle = (H\otimes H)(|\psi\rangle\otimes|\phi\rangle)$$
$$= (H|\psi\rangle)\otimes(H|\phi\rangle)$$

In particular,

$$H^{\otimes 2}|00\rangle = (H|0\rangle) \otimes (H|0\rangle)$$

$$= |+\rangle^{\otimes 2}$$

$$= \left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right]^{\otimes 2}$$

$$= \left(\frac{1}{\sqrt{2}}\right)^{2}(|0\rangle + |1\rangle)(|0\rangle + |1\rangle)$$

$$= \frac{1}{\sqrt{2^{2}}}(|00\rangle + |01\rangle + |10\rangle + |11\rangle).$$

Notice that this is an equal superposition of all possible values of the 2-qubit register. (I wrote the amplitude in a complicated way, $1/\sqrt{2^2}$, to help you see the general case.) In general,

$$H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}}(|0\rangle + |1\rangle)^{\otimes n}$$

$$= \frac{1}{\sqrt{2^n}}(|0\rangle + |1\rangle) \otimes (|0\rangle + |1\rangle) \otimes \cdots \otimes (|0\rangle + |1\rangle)$$

$$= \frac{1}{\sqrt{2^n}}(|00 \dots 00\rangle + |00 \dots 01\rangle + \cdots + |11 \dots 11\rangle)$$

$$= \frac{1}{\sqrt{2^n}} \sum_{\mathbf{x} \in 2^n} |\mathbf{x}\rangle$$

$$= \frac{1}{\sqrt{2^n}} \sum_{r=0}^{2^n-1} |\mathbf{x}\rangle.$$

Note that " 2^n-1 " represents a string of n 1-bits, and that $\mathbf{2}=\{0,1\}$. Hence, $H^{\otimes n}|0\rangle^{\otimes n}$ generates an equal superposition of all the 2^n possible values of the n-qubit register. We often write $W_n=H^{\otimes n}$ for the Walsh transformation.

An linear operation applied to such a superposition state in effect applies the operation simultaneously to all 2^n possible input values. This is *exponential* quantum parallelism and suggests that quantum computation might be able to solve exponential problems much more efficiently than classical computers. To see this, suppose $U|x\rangle = |f(x)\rangle$. Then:

$$U(H^{\otimes n}|0\rangle^{\otimes n}) = U\left[\frac{1}{\sqrt{2^n}}\sum_{x=0}^{2^n-1}|x\rangle\right] = \frac{1}{\sqrt{2^n}}\sum_{x=0}^{2^n-1}U|x\rangle = \frac{1}{\sqrt{2^n}}\sum_{x=0}^{2^n-1}|f(x)\rangle$$

This is a superposition of the function values f(x) for all of the 2^n possible values of x; it is computed by one pass through the operator U.

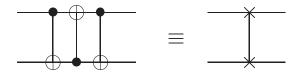


Figure III.11: Diagram for swap [from Nielsen & Chuang (2010)].

C.3 Quantum circuits

A quantum circuit is a sequential series of quantum transformations on a quantum register. The inputs are usually computational basis states (all $|0\rangle$ unless stated otherwise). Quantum circuit diagrams are drawn with time going from left to right, with the quantum gates crossing one or more "wires" (qubits) as appropriate. The circuit represents a sequence of unitary operations on a quantum register rather than physical wires.

These "circuits" are different in several respects from ordinary sequential logic circuits. First, loops (feedback) are not allowed, but you can apply transforms repeatedly. Second, FAN-IN (equivalent to OR) is not allowed, since it it not reversible or unitary. FAN-OUT is also not allowed, because it would violate the No-cloning Theorem. (N.B.: This does not contradict the universality of the Toffoli or Fredkin gates, which are universal only with respect to logical or classical states.)

Fig. III.9 (right) on page 104 shows the symbol for CNOT and its effect.

The swap operation is defined $|xy\rangle \mapsto |yx\rangle$, or explicitly

$$SWAP = \sum_{x,y \in \mathbf{2}} |yx \rangle \langle xy|.$$

We can put three CNOTs in series to swap two qubits (Exer. III.35). Swap has a special symbol as shown in Fig. III.11.

In general, any unitary operator U (on any number of qubits) can be conditionally controlled (see Fig. III.12); this is the quantum analogue of an if-then statement. If the control bit is 0, this operation does nothing, otherwise it does U. This is implemented by $|0\rangle\langle 0|\otimes I+|1\rangle\langle 1|\otimes U$. Effectively, the *operators* are entangled.

Suppose the control bit is in superposition, $|\chi\rangle = a|0\rangle + b|1\rangle$. The effect

111

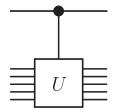


Figure 1.8. Controlled-U gate.

Figure III.12: Diagram for controlled-*U* [from Nielsen & Chuang (2010)].

of the conditional operation is:

$$(|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U)|\chi, \psi\rangle$$

$$= (|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U)(a|0\rangle + b|1\rangle) \otimes |\psi\rangle$$

$$= |0\rangle\langle 0|(a|0\rangle + b|1\rangle) \otimes I|\psi\rangle + |1\rangle\langle 1|(a|0\rangle + b|1\rangle) \otimes U|\psi\rangle$$

$$= a|0\rangle \otimes |\psi\rangle + b|1\rangle \otimes U|\psi\rangle$$

$$= a|0, \psi\rangle + b|1, U\psi\rangle.$$

The result is a superposition of entangled outputs. Notice that CNOT is a special case of this construction, a controlled X.

We also have a quantum analogue for an if-then-else construction. If U_0 and U_1 are unitary operators, then we can make the choice between them conditional on a control bit as follows:

$$|0\rangle\langle 0|\otimes U_0+|1\rangle\langle 1|\otimes U_1.$$

For example,

$$CNOT = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X.$$
 (III.17)

In quantum circuit diagrams, the symbol for the CCNOT gate is show in Fig. III.10, or with \bullet for top two connections and \oplus for bottom, suggesting CCNOT $|x,y,z\rangle=|x,y,xy\oplus z\rangle$. Alternately, put "CCNOT" in a box. Other operations may be shown by putting a letter or symbol in a box, for example "H" for the Hadamard gate.

The Hadamard gate can be used to generate Bell states (Exer. III.34):

$$CNOT(H \otimes I)|xy\rangle = |\beta_{xy}\rangle.$$
 (III.18)

In	Out	•
$ 00\rangle$	$(00\rangle + 11\rangle)/\sqrt{2} \equiv \beta_{00}\rangle$	<i>x</i> [11]
$ 01\rangle$	$(01\rangle + 10\rangle)/\sqrt{2} \equiv \beta_{01}\rangle$	
$ 10\rangle$	$(00\rangle - 11\rangle)/\sqrt{2} \equiv \beta_{10}\rangle$	$ \beta_{xy}\rangle$
$ 11\rangle$	$(00\rangle + 11\rangle)/\sqrt{2} \equiv \beta_{00}\rangle$ $(01\rangle + 10\rangle)/\sqrt{2} \equiv \beta_{01}\rangle$ $(00\rangle - 11\rangle)/\sqrt{2} \equiv \beta_{10}\rangle$ $(01\rangle - 10\rangle)/\sqrt{2} \equiv \beta_{11}\rangle$	$g \longrightarrow \oplus$

Figure III.13: Quantum circuit for generating Bell states. [from Nielsen & Chuang (2010, fig. 1.12)]

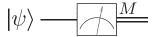


Figure III.14: Symbol for measurement of a quantum state (from Nielsen & Chuang (2010)).

The circuit for generating Bell states (Eq. III.18) is shown in Fig. III.13. It's also convenient to have a symbol for quantum state measurement, such as Fig. III.14.

C.4 Quantum gate arrays

Fig. III.15 shows a quantum circuit for a 1-bit full adder. As we will see (Sec. C.7), it is possible to construct reversible quantum gates for any classically computable function. In particular the Fredkin and Toffoli gates are universal.

Because quantum computation is a unitary operator, it must be reversible. You know that an irreversible computation $x \mapsto f(x)$ can be embedded in a reversible computation $(x,c)\mapsto (g(x),f(x))$, where c are suitable ancillary constants and g(x) represents the garbage qubits. Note that throwing away the garbage qubits (dumping them into the environment) will collapse the quantum state (equivalent to measurement) by entangling them in the many degrees of freedom of the environment. Typically these garbage qubits will be entangled with other qubits in the computation, collapsing them as well, and interfering with the computation. Therefore the garbage

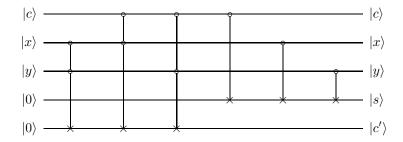


Figure III.15: Quantum circuit for 1-bit full adder [from Rieffel & Polak (2000)]. "x and y are the data bits, s is their sum (modulo 2), c is the incoming carry bit, and c' is the new carry bit."

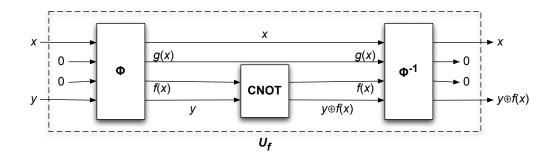


Figure III.16: Quantum gate array for reversible quantum computation.

must be produced in a *standard state* independent of x. This is accomplished by uncomputing, as we did in classical reversible computing (Ch. II, Sec. C.6, p. 57).

Since NOT is reversible, each 1 bit in c can be replaced by a 0 bit followed by a NOT, so we need only consider computations of the form $(x,0) \mapsto (g(x), f(x))$; that is, all the constant bits can be zero.

Therefore, we begin by embedding our irreversible computation of f in a reversible computation Φ , which we get by providing 0 constants and generating garbage g(x); see Fig. III.16. That is, Φ will perform the following computation on four registers (data, workspace, result, target):

$$(x, 0, 0, y) \mapsto (x, g(x), f(x), y).$$

The result f(x) is in the result register and the garbage g(x) is in the workspace register. Notice that x and y (data and target) are passed through. Now use CNOTs between corresponding places in the result and target registers to compute $y \oplus f(x)$, where \oplus represents bitwise exclusive-or, in the target register. Thus we have computed:

$$(x,0,0,y)\mapsto (x,g(x),f(x),y\oplus f(x)).$$

Now we uncompute with Φ^{-1} , but since the data and target registers are passed through, we get $(x,0,0,y\oplus f(x))$ in the registers. We have restored the data, workspace, and result registers to their initial values and have $y\oplus f(x)$ in the target register. Ignoring the result and workspace registers, we write

$$(x,y)\mapsto (x,y\oplus f(x)).$$

This is the standard approach we will use for embedding a classical computation in a quantum computation.

Therefore, for any computable $f: \mathbf{2}^m \to \mathbf{2}^n$, there is a reversible quantum gate array $U_f: \mathcal{H}^{m+n} \to \mathcal{H}^{m+n}$ such that for $x \in \mathbf{2}^m$ and $y \in \mathbf{2}^n$,

$$U_f|x,y\rangle = |x,y \oplus f(x)\rangle,$$

See Fig. III.17. In particular, $U_f|x, \mathbf{0}\rangle = |x, f(x)\rangle$. The first m qubits are called the *data register* and the last n are called the *target register*.

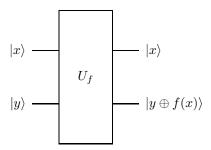


Figure III.17: Computation of function by quantum gate array (Rieffel & Polak, 2000).

C.5 Quantum parallelism

Since U_f is linear, if it is applied to a superposition of bit strings, it will produce a superposition of the results of applying f to them in parallel (i.e., in the same time it takes to compute it on one input):

$$U_f(c_1|\mathbf{x}_1\rangle + c_2|\mathbf{x}_2\rangle + \dots + c_k|\mathbf{x}_k\rangle) = c_1U_f|\mathbf{x}_1\rangle + c_2U_f|\mathbf{x}_2\rangle + \dots + c_kU_f|\mathbf{x}_k\rangle.$$

For example, if we have a superposition of the inputs \mathbf{x}_1 and \mathbf{x}_2 ,

$$U_f\left(\frac{\sqrt{3}}{2}|\mathbf{x}_1\rangle + \frac{1}{2}|\mathbf{x}_2\rangle\right) \otimes |\mathbf{0}\rangle = \frac{\sqrt{3}}{2}|\mathbf{x}_1, f(\mathbf{x}_1)\rangle + \frac{1}{2}|\mathbf{x}_2, f(\mathbf{x}_2)\rangle.$$

The amplitude of a result y will be the sum of the amplitudes of all x such that y = f(x).

If we apply U_f to a superposition of all possible 2^m inputs, it will compute a superposition of all the corresponding outputs in parallel (i.e., in the same time as required for one function evaluation)! The Walsh-Hadamard transformation can be used to produce this superposition of all possible inputs:

$$W_{m}|00...0\rangle = \frac{1}{\sqrt{2^{m}}} (|00...0\rangle + |00...1\rangle + \cdots + |11...1\rangle)$$

$$= \frac{1}{\sqrt{2^{m}}} \sum_{\mathbf{x} \in \mathbf{2}^{m}} |\mathbf{x}\rangle$$

$$= \frac{1}{\sqrt{2^{m}}} \sum_{x=0}^{2^{m}-1} |x\rangle.$$

In the last line we are obviously interpreting the bit strings as natural numbers. Hence,

$$U_f W_m |\mathbf{0}\rangle = U_f \left(\frac{1}{\sqrt{2^m}} \sum_{x=0}^{2^m - 1} |x, 0\rangle \right) = \frac{1}{\sqrt{2^m}} \sum_{x=0}^{2^m - 1} U_f |x, 0\rangle = \frac{1}{\sqrt{2^m}} \sum_{x=0}^{2^m - 1} |x, f(x)\rangle.$$

A single circuit does all 2^m computations simultaneously! "Note that since n qubits enable working simultaneously with 2^n states, quantum parallelism circumvents the time/space trade-off of classical parallelism through its ability to provide an exponential amount of computational space in a linear amount of physical space." (Rieffel & Polak, 2000)

This is amazing, but not immediately useful. If we measure the input bits, we will get a random value, and the state will be projected into a superposition of the outputs for the inputs we measured. If we measure an output bit, we will get a value probabilistically, and a superposition of all the inputs that can produce the measured output. Neither of the above is especially useful, so most quantum algorithms transform the state in such a way that the values of interest have a high probability of being measured. The other thing we can do is to extract common properties of all values of f(x). Both of these require different programming techniques than classical computing.