

Ancilla management for quantum and reversible computation

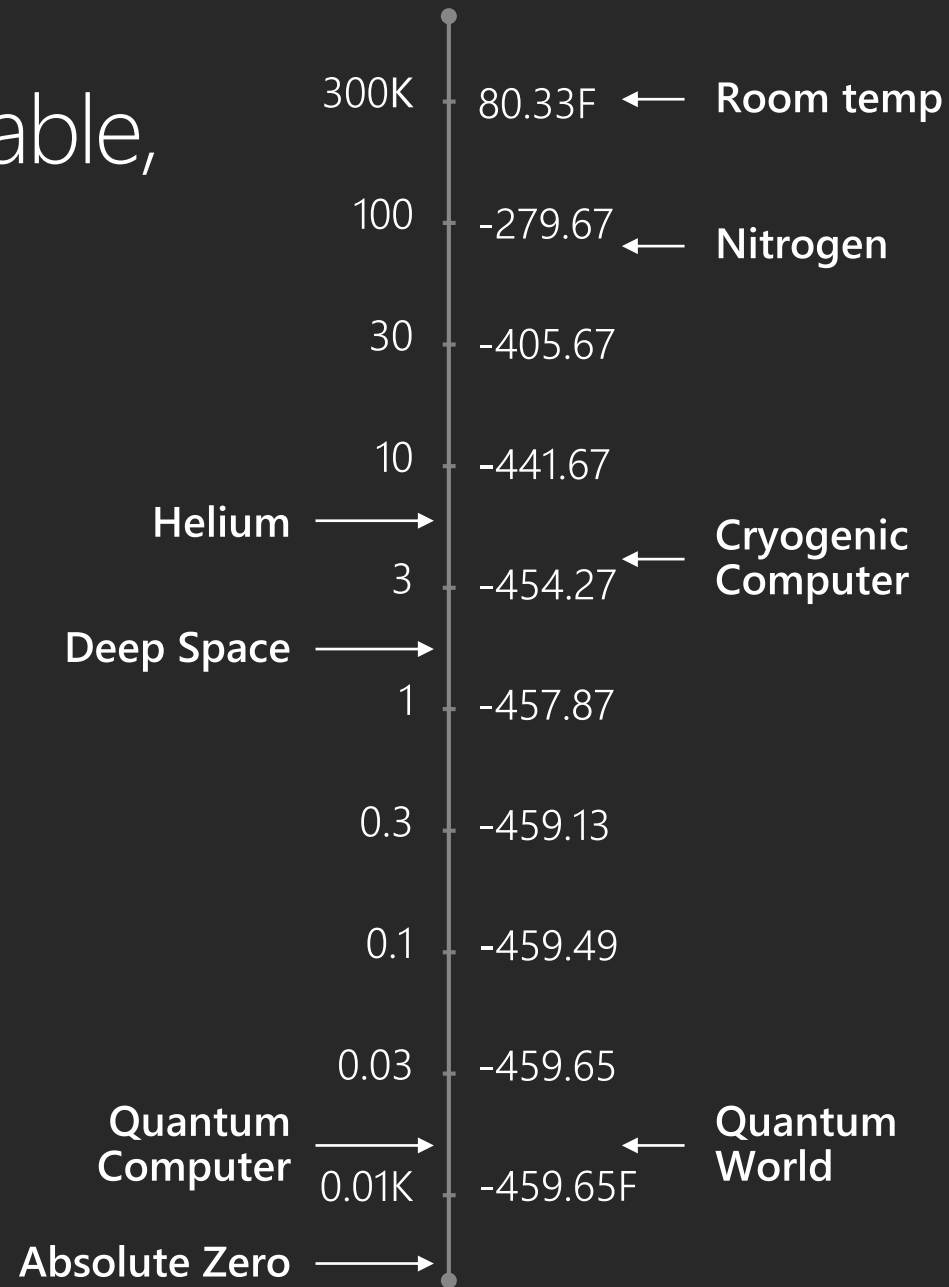
Martin Roetteler
Microsoft Research



Igniting a quantum revolution



A complete, scalable, quantum system



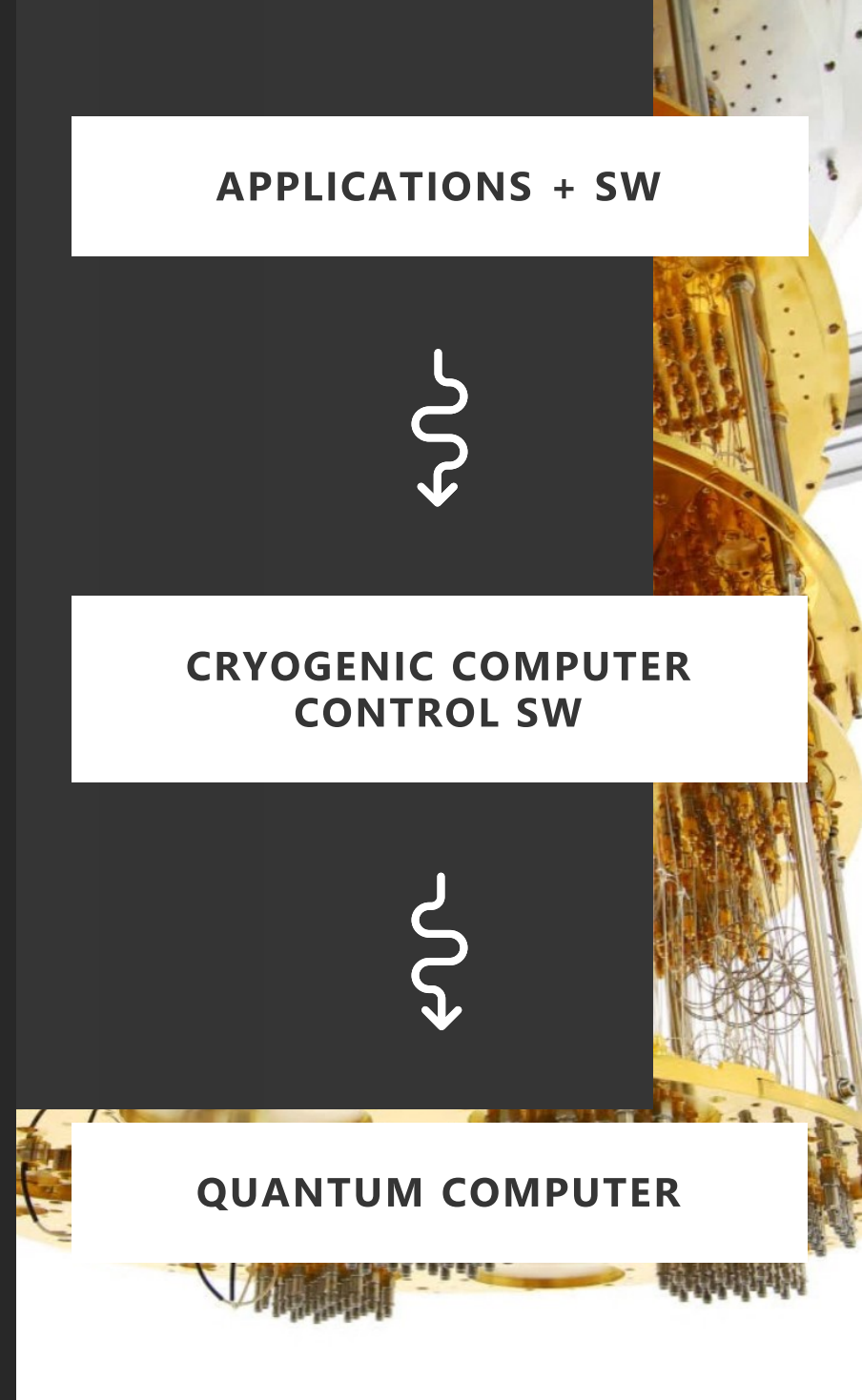
APPLICATIONS + SW



CRYOGENIC COMPUTER CONTROL SW



QUANTUM COMPUTER



Nitrogen
fixation

Carbon
capture

Materials
science

Machine
learning

Quantum "Hello, World"

```
HelloWorld-e2e - Microsoft Visual Studio
File Edit View Project Build Debug Team Tools Architecture Test Analyze Window Help
Debug Any CPU Start
Teleport.qb x Teleport.g.cs
1 operation () EPR (Qubit q1, Qubit q2) {
2     Body {
3         H (q1)
4         CNOT (q1,q2)
5     }
6 }
7
8 operation () Teleport (Qubit msg, Qubit here, Qubit there) {
9     Body {
10        EPR (here, there)
11        CNOT (msg, here)
12        H (msg)
13
14        let m_here = M (here)
15        if (m_here == One) {
16            X (there)
17        }
18
19        let m_msg = M (msg)
20        if (m_msg == One) {
21            Z (there)
22        }
23    }
24 }
25
26 operation (Result) TeleportTest (Result msg) {
27     Body {
28         mutable res = Zero
29         using (qubits = Qubit[3]) {
30             let msgQ = qubits[0]
31
32             // Set msgQ to message state
33             SetQubit (msg, msgQ)
34
35             Teleport (msgQ, qubits[1], qubits[2])
36
37             set res = M (qubits[2])
38         }
39         return res
40     }
41 }
42
```

Overview

Quantum entanglement and interference

Reversible computing

- Avoiding garbage by “un”-computing

- Design space exploration

Quantum memory management

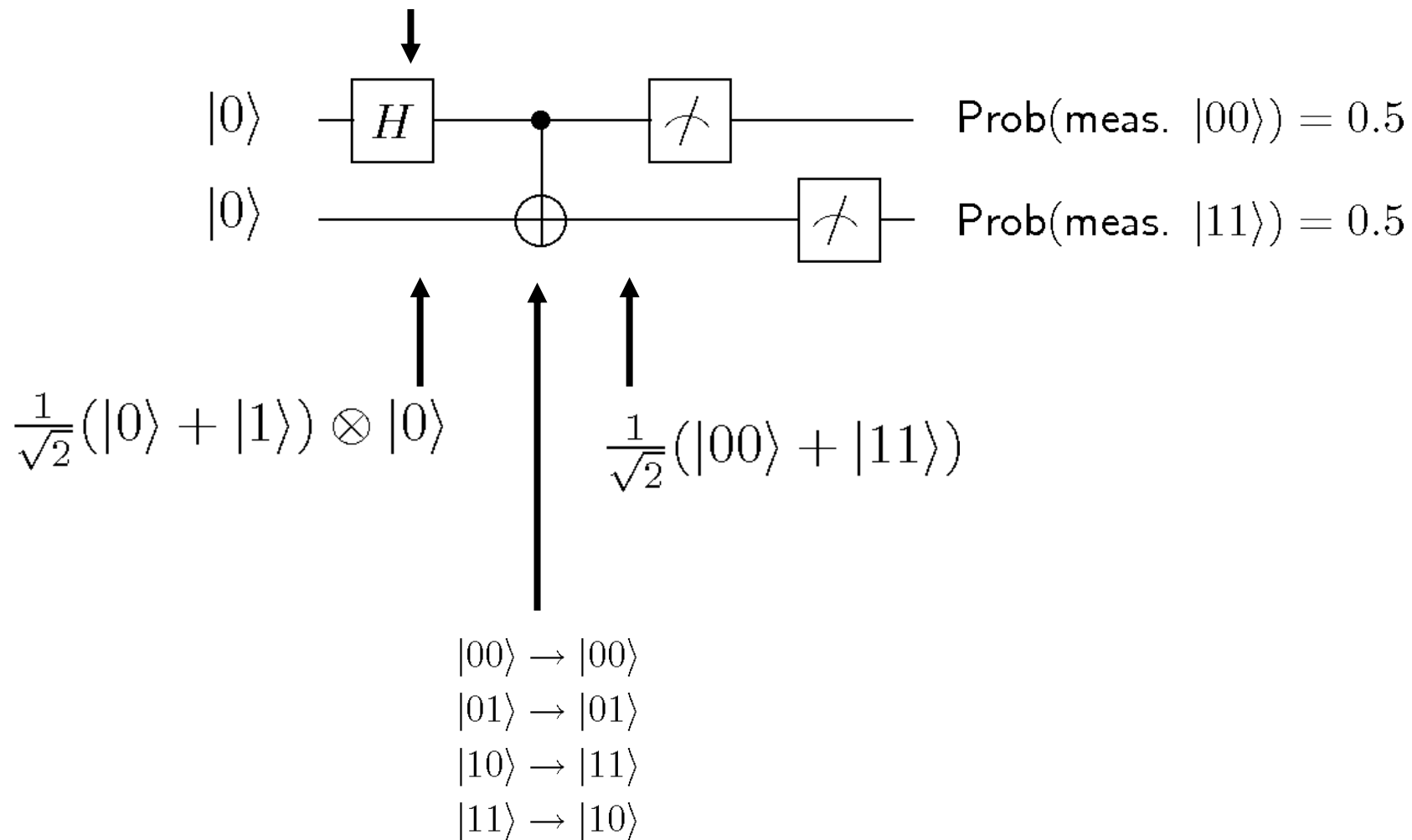
- Working with “dirty” qubits

Cryptanalysis of ECC signatures

- Libraries for modular arithmetic

Quantum circuit example

$$H \otimes \mathbf{1}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \mathbf{1}_2$$



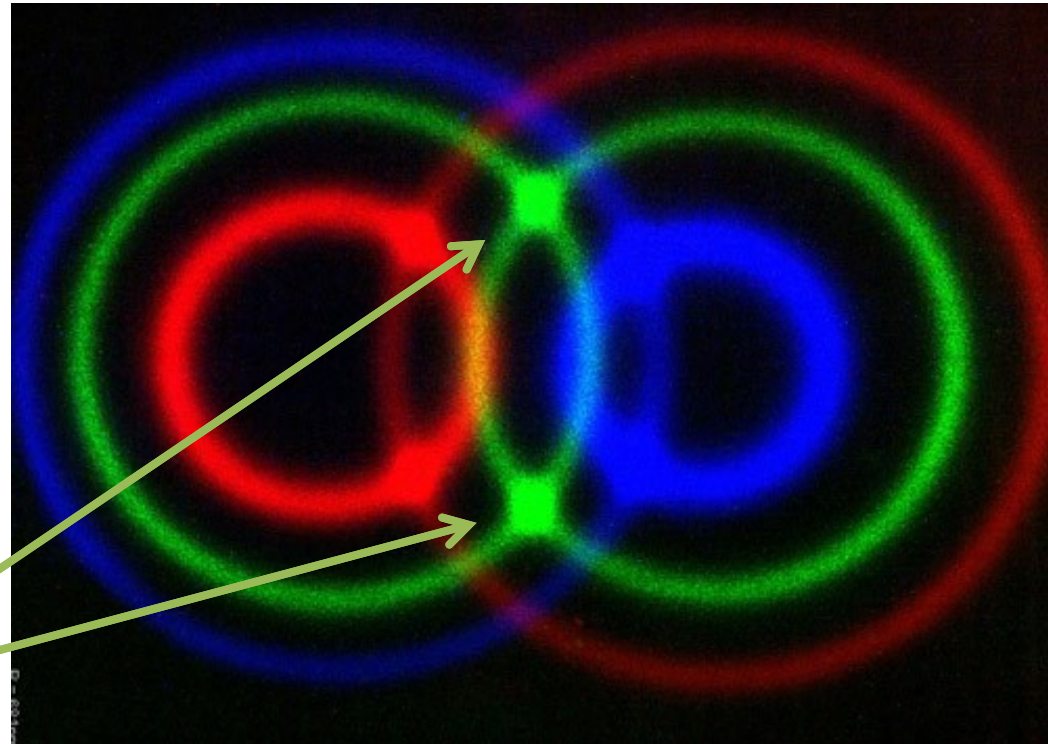
Entangled states

- States that cannot be characterized using only local correlations
- Example: the EPR state $\frac{|01\rangle - |10\rangle}{\sqrt{2}}$ (after Einstein, Podolsky, and Rosen)

(also called “EPR pair”)

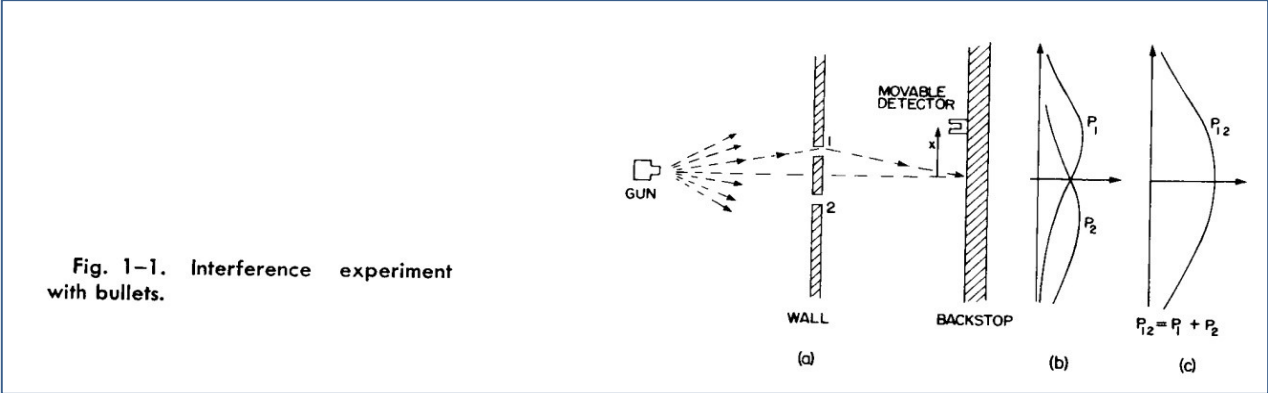
- In optics, EPR pairs can be generated e.g. using parametric downconversion

Entangled state between photons emitted with same wavelength (i.e., same color) but with orthogonal polarizations H and V. At the intersection points the polarization is undefined, but different, resulting in a state of the form $1/\sqrt{2}(|H\rangle|V\rangle + e^{i\alpha}|V\rangle|H\rangle)$.

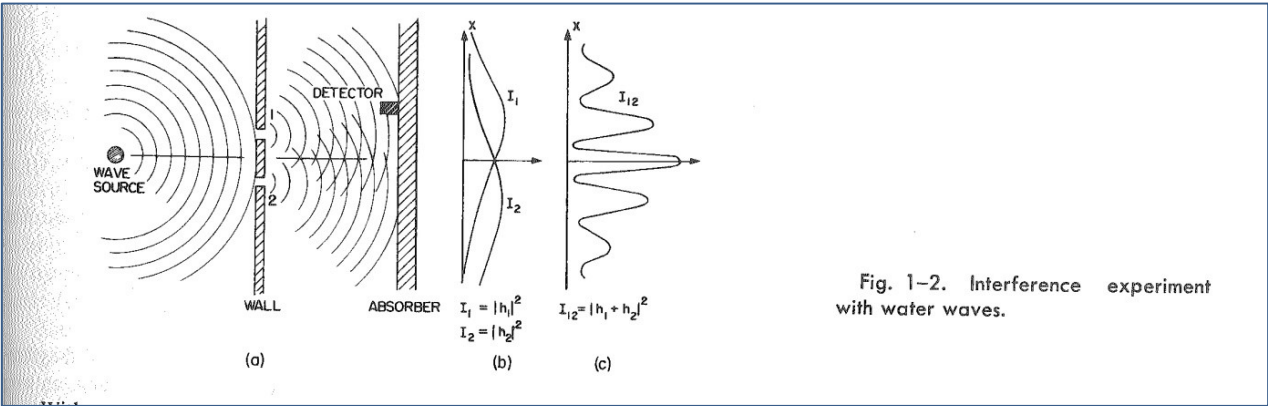


Interference: the double-slit experiment

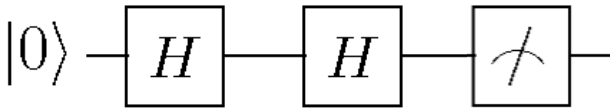
Experiment A (“Lee Marvin style”): a gun shoots bullets through 2 holes. Probability for outcome at x is given by summation of two probabilities.



Experiment B (“Water waves”): a source emits water waves. Probability for final outcome at point x also depends on **phases** of incoming waves.



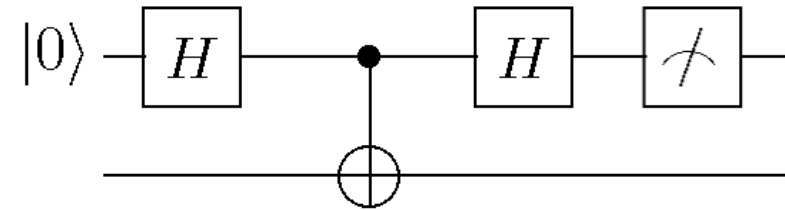
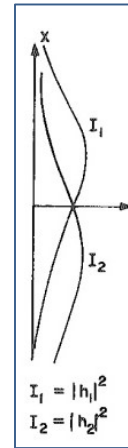
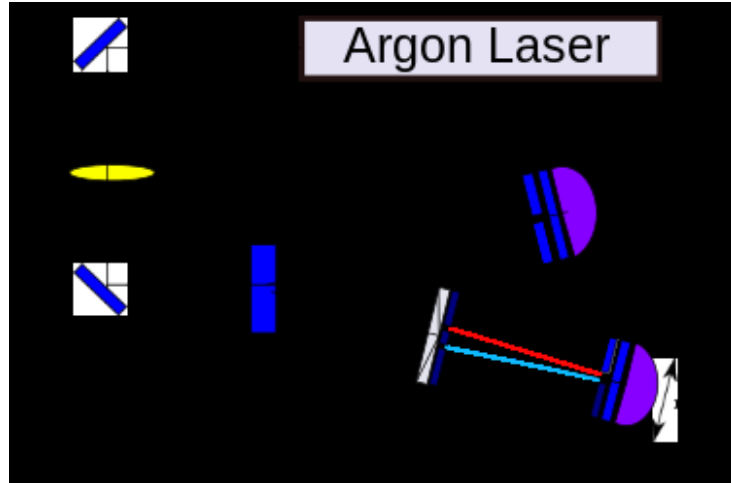
Interference example as circuit:



[Pictures credit: R. Feynman, FLP vol I]

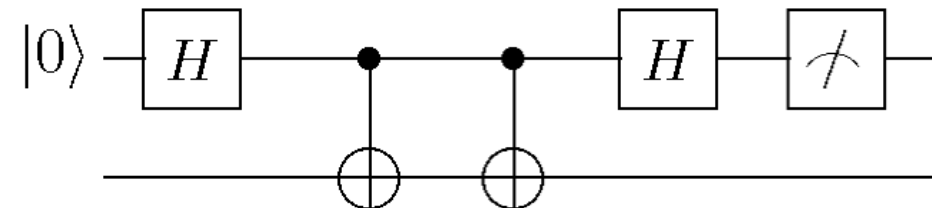
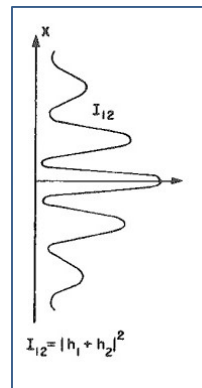
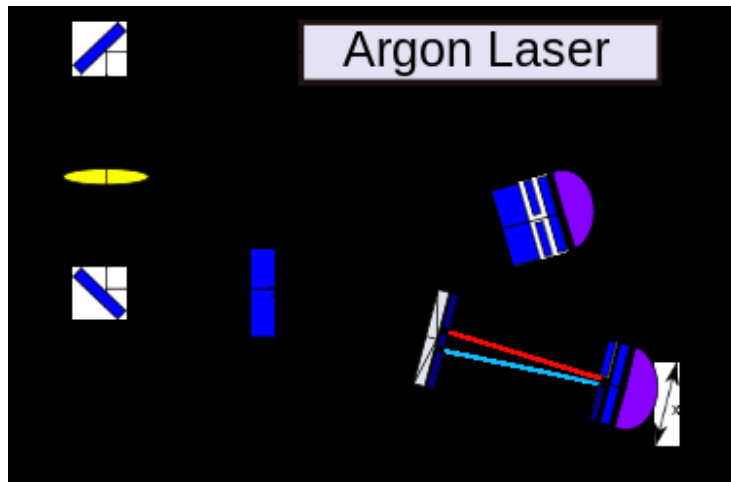
Why garbage is fatal for interference

- By inserting polarization filters, the paths can be made distinguishable. The interference pattern disappears.



Example using reversible functions:
 $|x\rangle|0\rangle|0\rangle \mapsto |x\rangle|f(x)\rangle|g(x)\rangle$

- Quantum eraser experiment: ([Wheeler '78], [Scully et al, '82 and '99]): "Erase" polarization information **after** the photon passed the slits. The interference pattern re-appears!



Example using reversible functions:
 $|x\rangle|0\rangle|0\rangle \mapsto |x\rangle|f(x)\rangle|0\rangle$

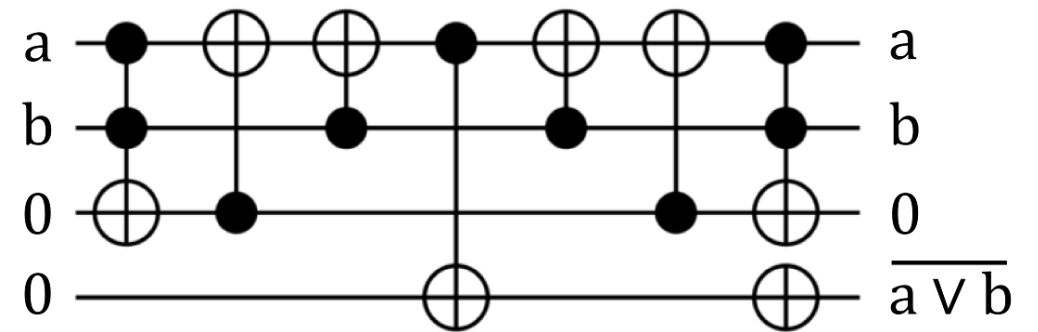
Reversible computing: why do we care?

- Arithmetic:
 - Factoring: just needs “constant” modular arithmetic
 - ECC dlogs: need generic modular arithmetic
 - HHL: need integer inverses; Newton type methods
- Amplitude amplification:
 - Implementation of the “oracles”, e.g., for search, collision etc.
 - Implementation of walk operators on data structures
- Quantum simulation:
 - Addressing/indexing functions for sparse matrices
 - Computing Hamiltonian terms on the fly

Universal reversible gate set: Toffoli gates

Fact: The set {Toffoli, CNOT, NOT} is universal for reversible computing: any *even* permutation on n qubits can be written as a sequence of Toffoli, CNOT, and NOT gates. [Toffoli'80], [Fredkin/Toffoli'82]

Example:

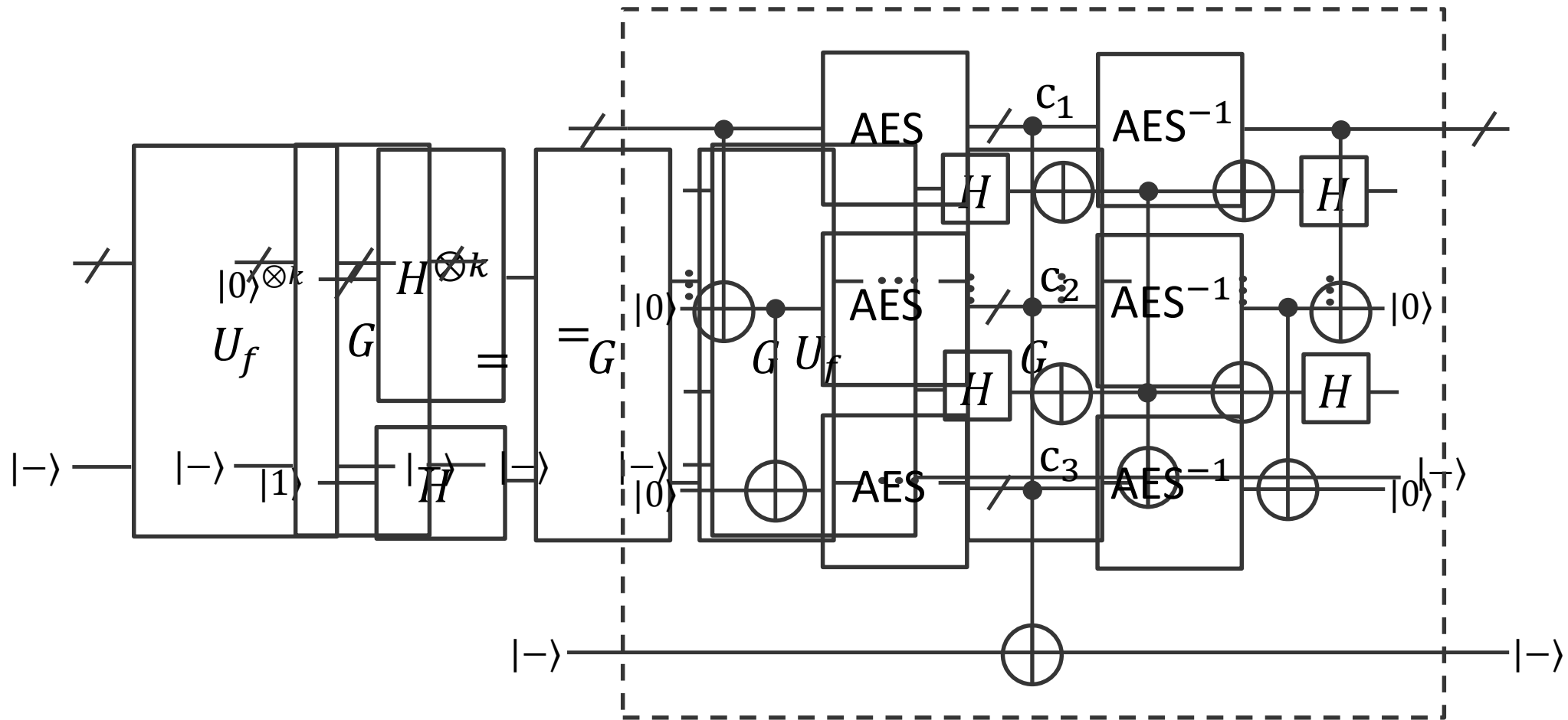


Main motivation: How can we find efficient implementations of reversible circuits in terms of efficient Toffoli networks?

How can we do this starting from irreversible descriptions in a programming language like Python or Haskell or F# or C?

Can we trade time (circuit depth) for space (#qubits) in a meaningful way?

Zooming into a quantum algorithm: Grover



[Grassl, Langenberg, R., Steinwandt, PQCrypto'16]

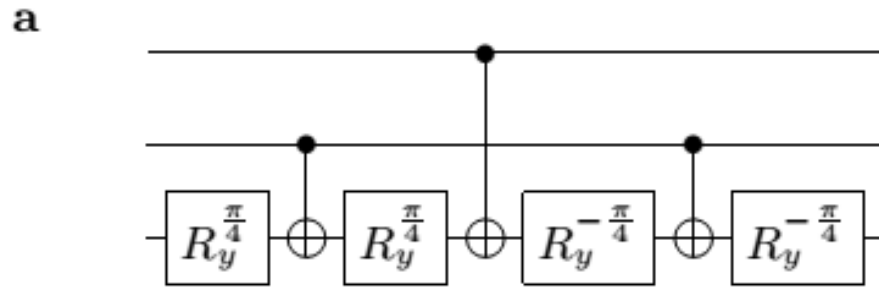
$$f(K) := (AES_K(m_1) = c_1) \wedge \dots \wedge (AES_K(m_r) = c_r)$$

An example at scale: SHA-2

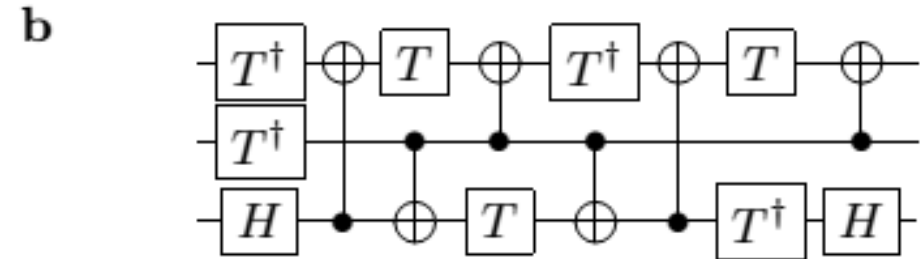
Hash function:

```
Initialize hash values
h0 := 0x6a09e667
h1 := 0xbb67ae85
...
h7 := 0x5be0cd19
Initialize constants
k[0..63] := 0x428a2f98, 0x71374491, 0xb5c0fbcf, ...
Do preprocessing
break message into 512-bit chunks (16 32bit ints)
Expand to 64 32 bit ints as follows:
Create W: a 64 entry array of 32 bit ints
Copy the message into w[0..15] and do:
for each chunk
    for i from 16 to 63
        s0 := (w[i-15] >> 7) ⊕ (w[i-15] >> 18) ⊕ (w[i-15] >> 3)
        s1 := (w[i-2] >> 17) ⊕ (w[i-2] >> 19) ⊕ (w[i-2] rshift 10)
        w[i] := w[i-16] + s0 + w[i-7] + s1
    Initialize working variables to current hash value:
    a := h0
    ...
    h := h7 Compression function main loop:
    Do compression rounds
    Add the compressed chunk to the current hash value:
    h0 := h0 + a
    ...
    h7 := h7 + h
digest := hash := h0 :: h1 :: h2 :: h3 :: h4 :: h5 :: h6 :: h7
```

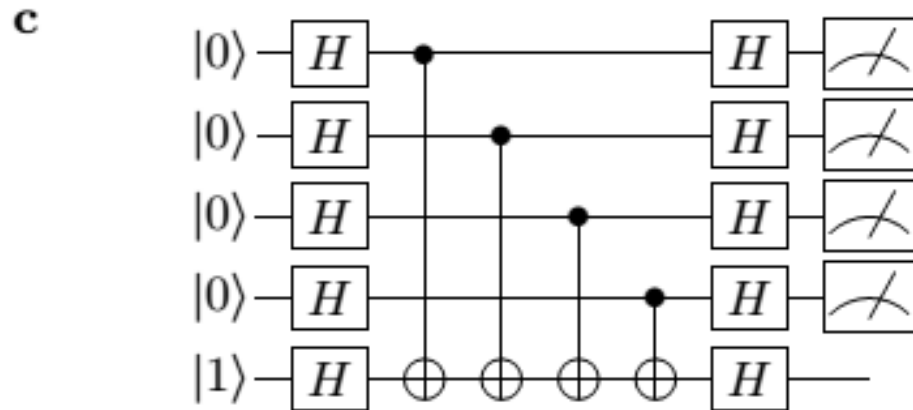

Benchmark "algorithms"



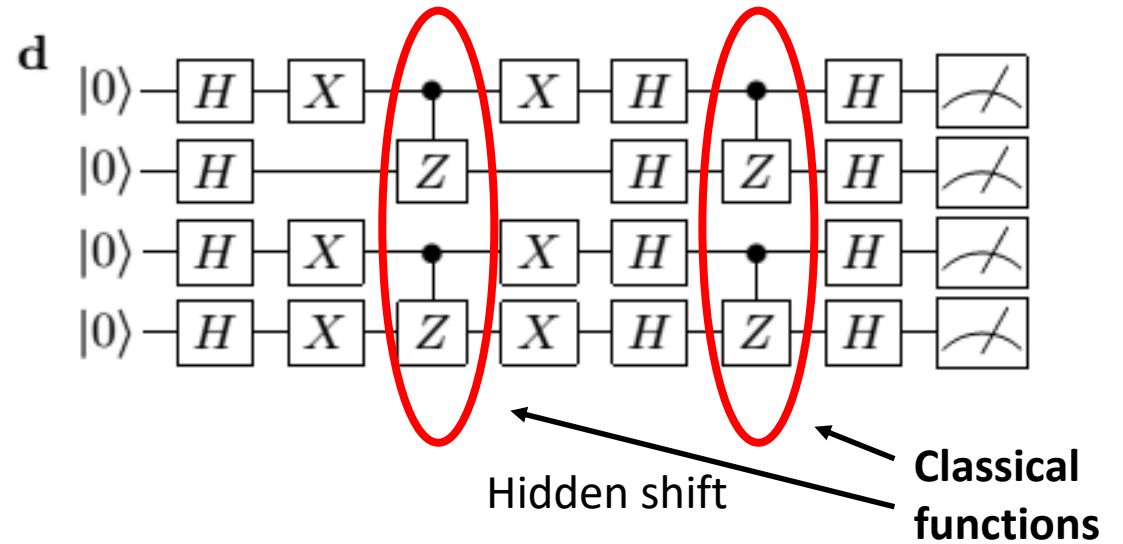
Margolus gate



Toffoli gate

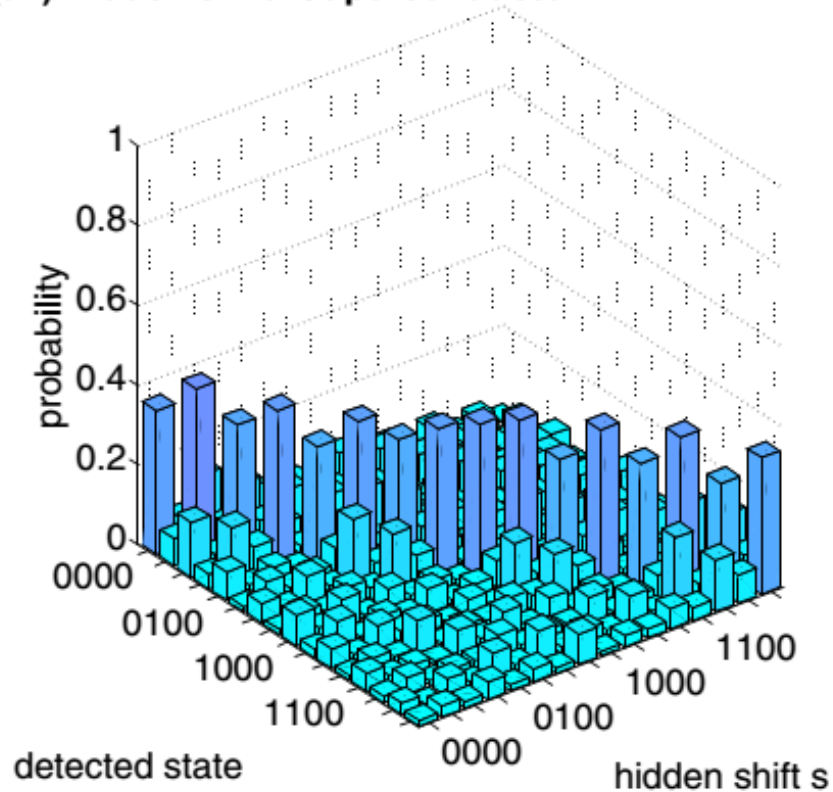


Bernstein-Vazirani



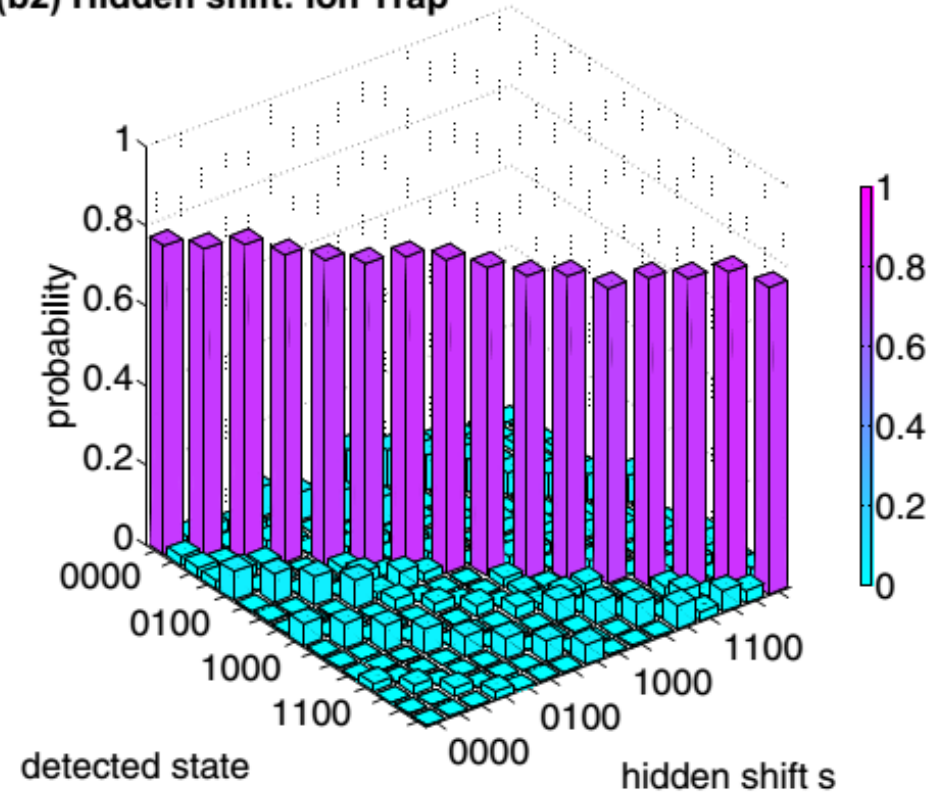
Experiments on quantum HW: hidden shifts

(a2) Hidden shift: Superconductor



$$\overline{P}_{success} = 0.35$$

(b2) Hidden shift: Ion Trap

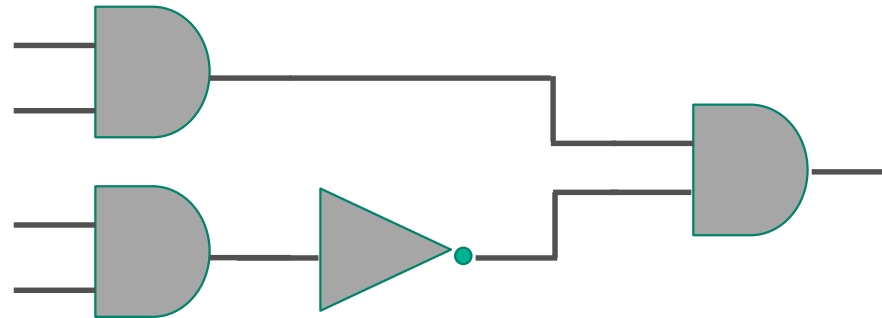


$$\overline{P}_{success} = 0.77$$

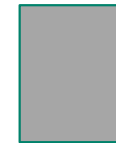
[Linke et al, Proc. Nat. Acad. Science, 2017]

Reversible embeddings

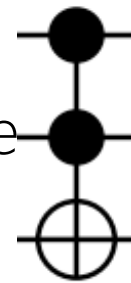
Example:



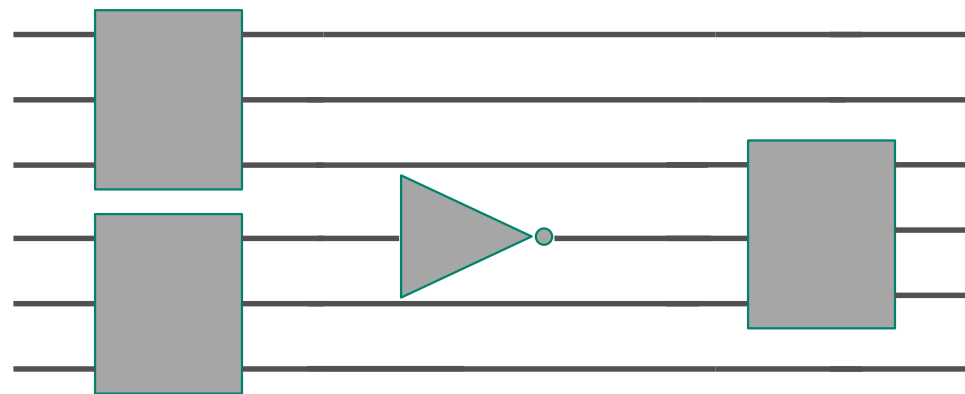
Replace each gate with a reversible one: (e.g.,



= Toffoli gate



)



How to avoid garbage?

- Replacing each gate with a reversible one works fine, however, it produces “garbage”, i.e., help registers will be in a state different from 0 at the end.
- There is a way out of this dilemma: the Bennett trick

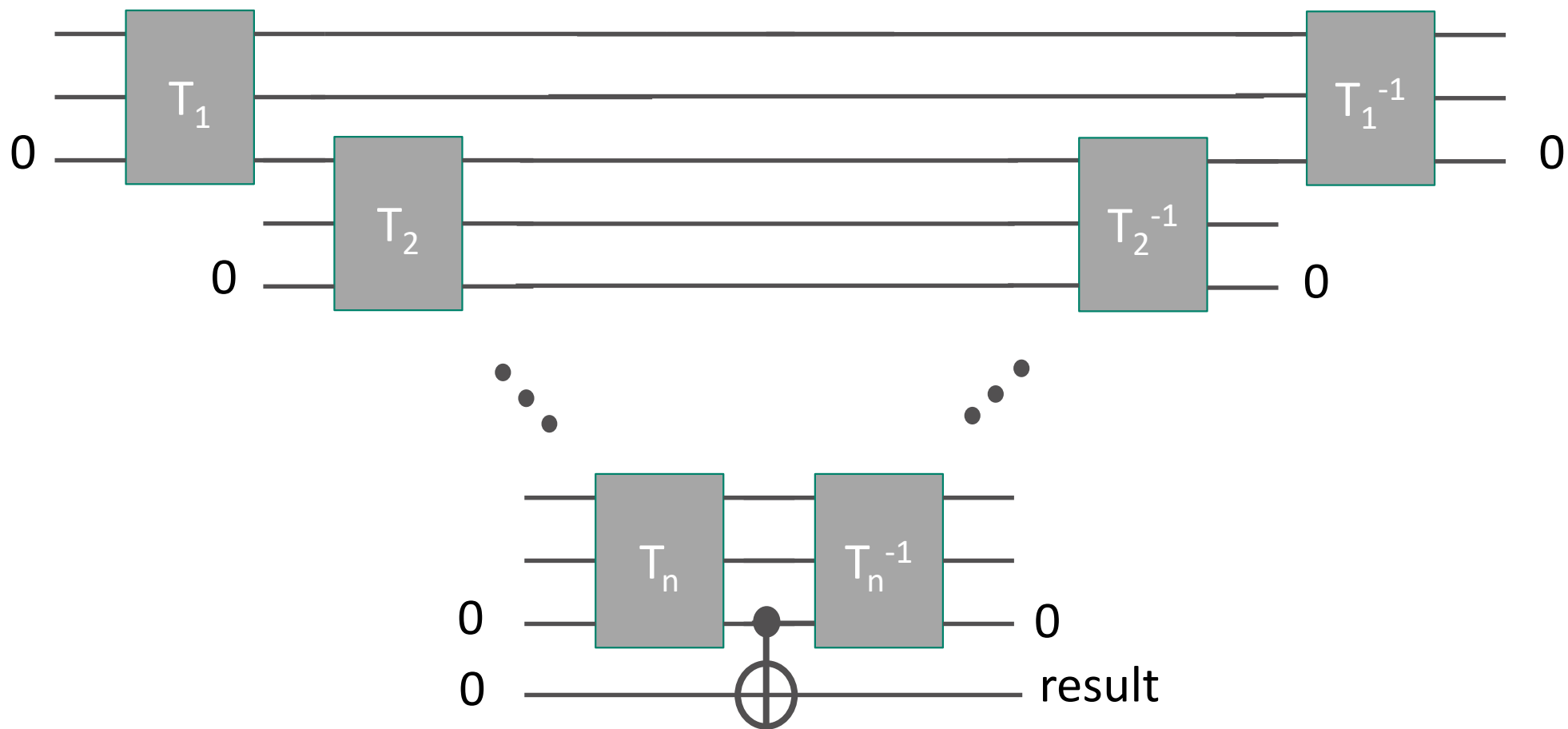
$$\begin{aligned} |x\rangle |0\rangle |0\rangle |0\rangle &\mapsto |x\rangle |f(x)\rangle |garbage(x)\rangle |0\rangle \\ &\mapsto |x\rangle |f(x)\rangle |garbage(x)\rangle |f(x)\rangle \\ &\mapsto |x\rangle |0\rangle |0\rangle |f(x)\rangle \end{aligned}$$

Idea: compute forward, copy the result, “uncompute” the garbage by running the computation backwards.

Problem: this leads to a large quantum memory footprint.

Cleaning up the ancilla (scratch) qubits

- Replace each gate with a reversible one [Bennett, IBM JRD'73]:

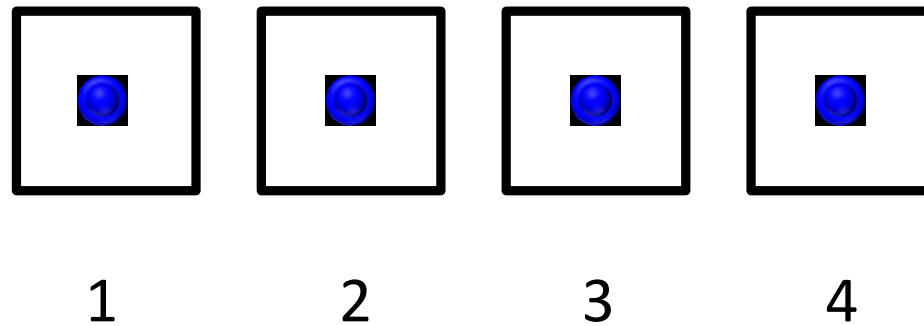


Pebble game: case of 1D chain

Rules of the game: [\[Bennett, SIAM J. Comp., 1989\]](#)

- n boxes, labeled $i = 1, \dots, n$
- in each move, either add or remove a pebble
- a pebble can be added or removed in $i=1$ at any time
- a pebble can be added or removed in $i>1$ if and only if there is a pebble in $i-1$
- 1D nature arises from decomposing a computation into “stages”

Example:



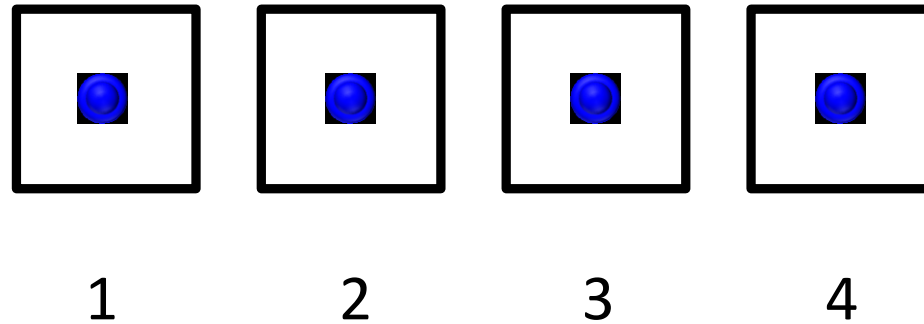
#	i
1	1
2	2
3	3
4	4
5	3
6	2
7	1

Pebble game: 1D chain w/space constraints

Imposing resource constraints:

- only a total of S pebbles are allowed
- corresponds to reversible algorithm with at most S ancilla qubits

Example: $(n=3, S=3)$

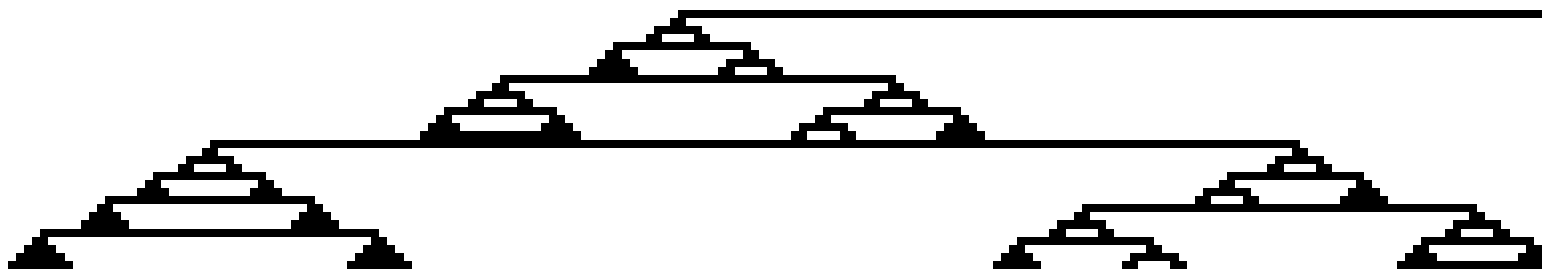
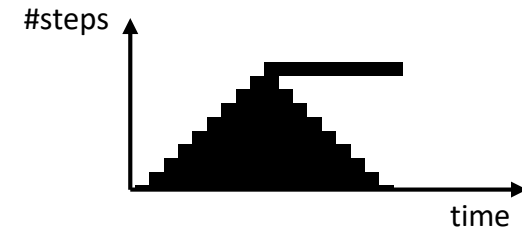


#	i
1	1
2	2
3	3
4	1
5	4
6	3
7	1
8	2
9	1

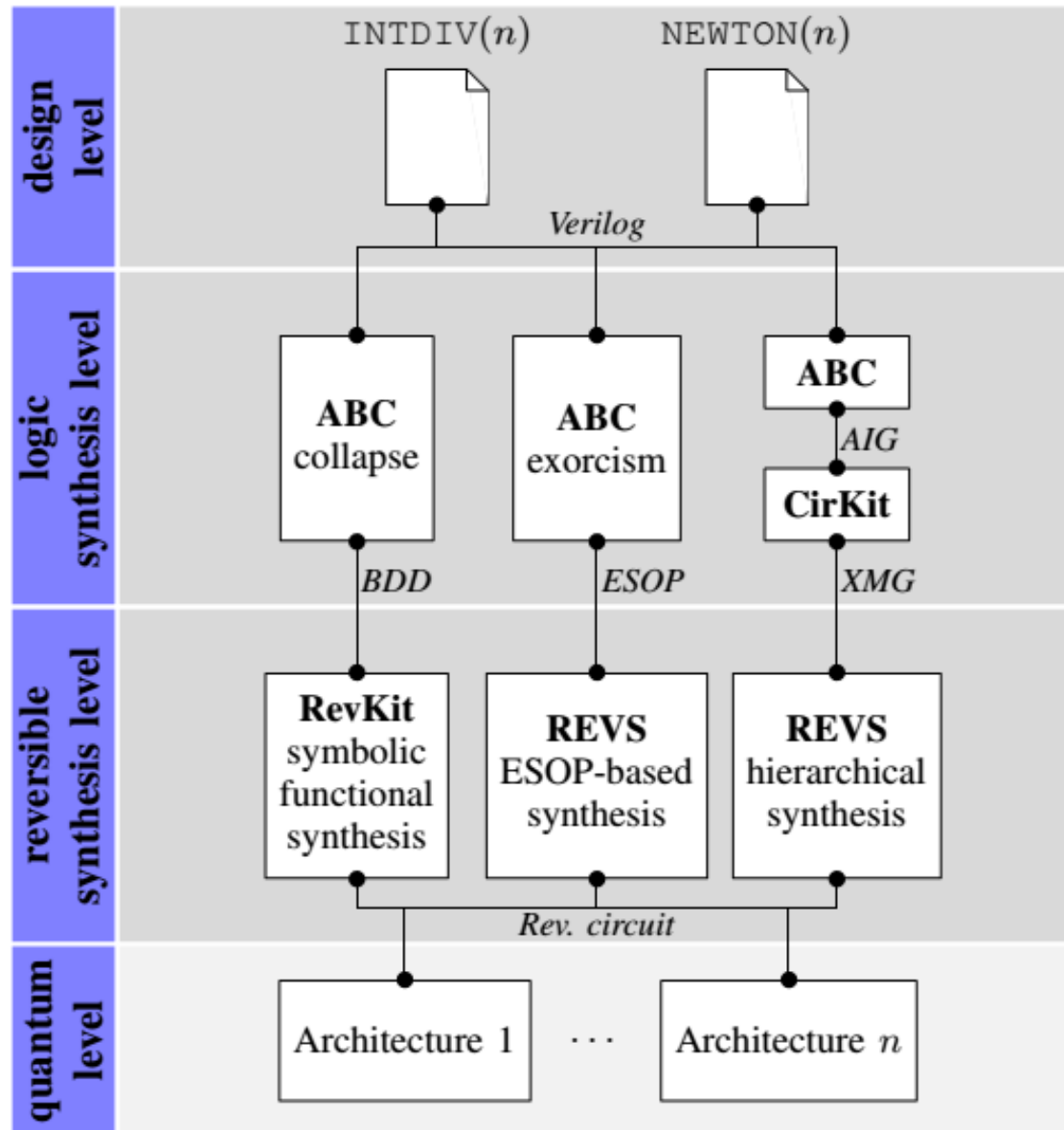
Optimal pebbling strategies: 1D chains

Dynamic programming: Allows to find best strategy for given number of steps n to be performed and given space resource constraint S which is the number of available pebbles.

This works ok for 1D chains. For general graphs the problem of finding the optimal strategy is difficult (PSPACE complete problem) -> need heuristics



Circuit synthesis for classical subroutines



Example: compute integer division $x \mapsto 2^n/x$,
Where x is an n -bit (unsigned) integer and the result is rounded to the closest integer.

At design level: start from high-level implementations of division function in Verilog. We considered:

- Integer long division (divide $2^n = qx + r$)
- Newton-Raphson

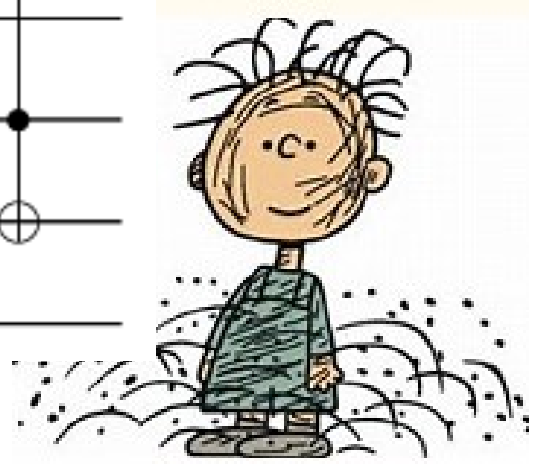
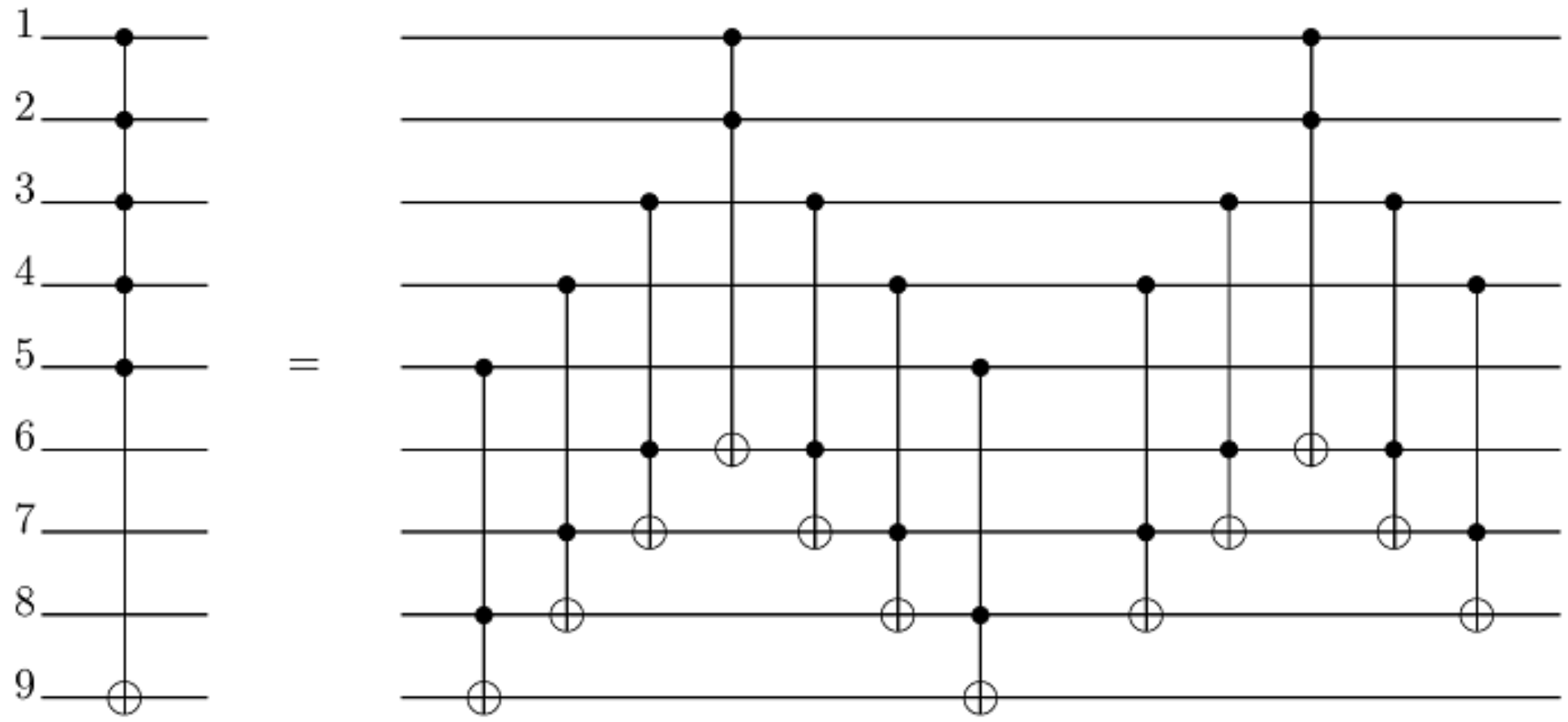
At logic synthesis level:

- Convert Verilog to logical netlist in AIG format (And-Inverter Graphs) using tool ABC
- Convert AIG to ESOP format (Exclusive Sums of Products) using tool XOR-cism
- Convert ESOP to Toffoli networks using different tools (REVS, RevKit)
- Also, we considered LUT based synthesis

Several passes through the above for various parameter settings that allow T-count/space/compile time tradeoffs.

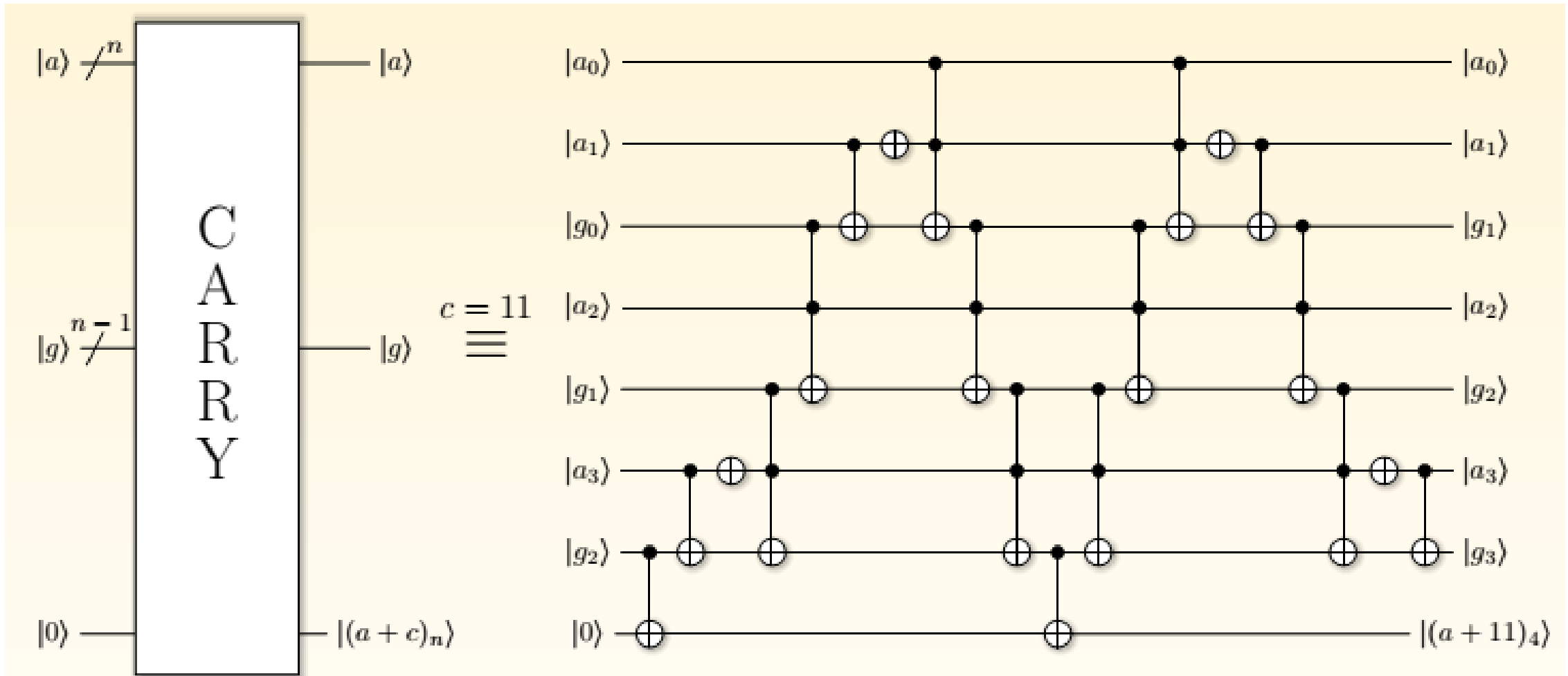
Dirty qubits

Implementation of Shor's algorithm on $2n+2$ qubits



Basic inspiration: apply tricks similar to the above to use “dirty” ancillas for optimization (Barenco et al, PRA'95)

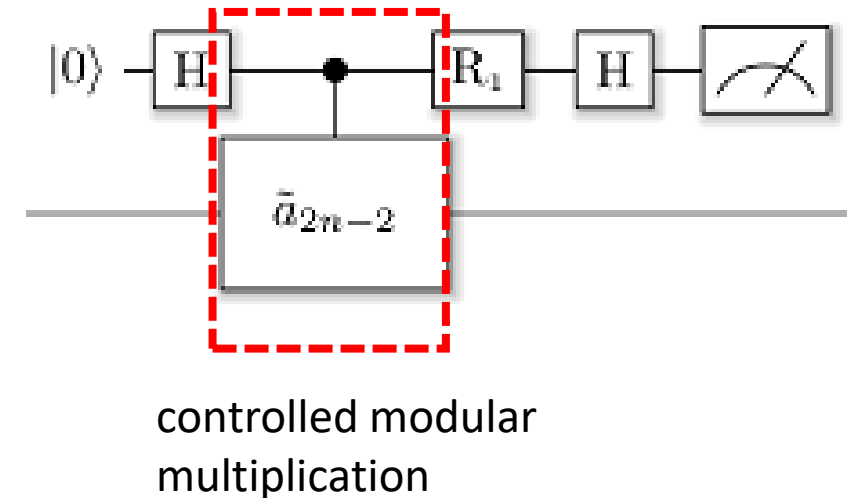
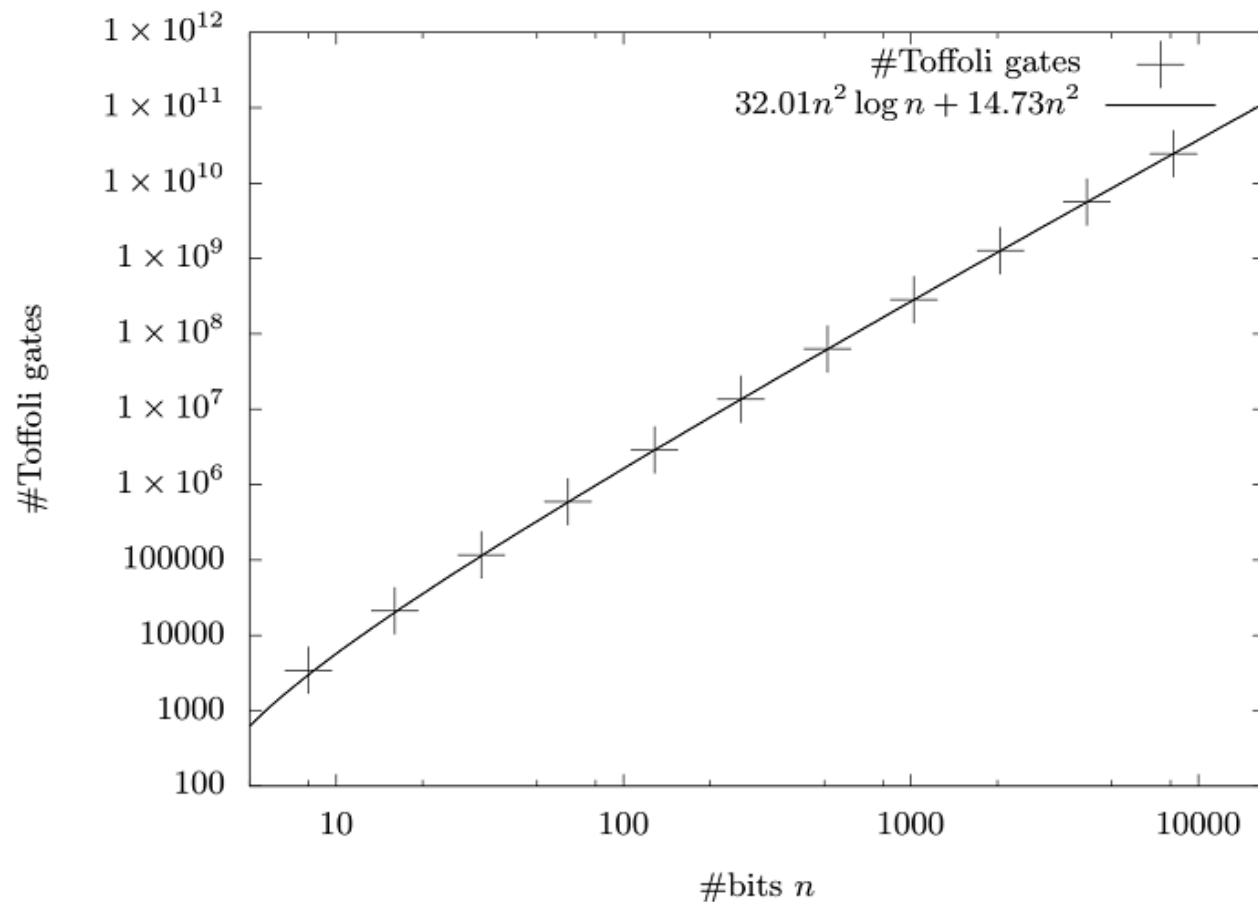
Carry prediction with dirty ancillas



[Haener, R., Svore, QIC 2017]
 [Gidney, arXiv:1706.07884]

Based on this, one can build constant folded modular arithmetic (+, *, exp)

Simulating the entire modular multiplication



[Haener, R., Svore, QIC 2017]

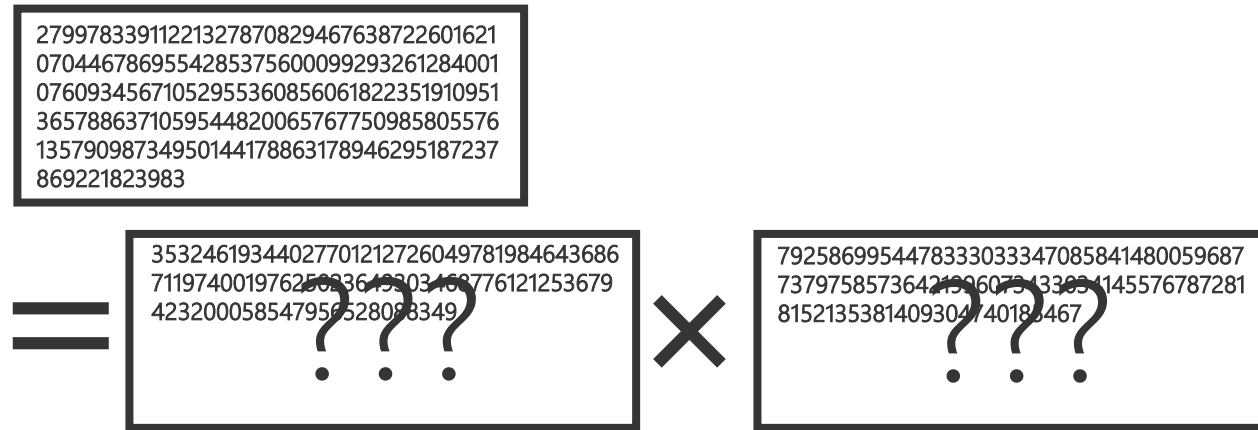
- Built Toffoli network for modular-multiplication for bit sizes relevant for RSA (1024-8192)
- Simulated networks in LIQUi|> using Toffoli simulator
- Metrics for entire Shor algorithm: #qubits = $2n + 2$, #Toffoli-gates = $64n^3 \log(n) + 29.45n^3$

Breaking ECC crypto

Or: why we need powerful quantum software libraries

Breaking RSA and elliptic curve signatures

Integer factorization



Best known methods to factor n -bit numbers*:

Classical: $O(\exp(c n^{1/3} (\log n)^{2/3}))$

Quantum: $O(n^2 \log n 2^{\log^* n})$

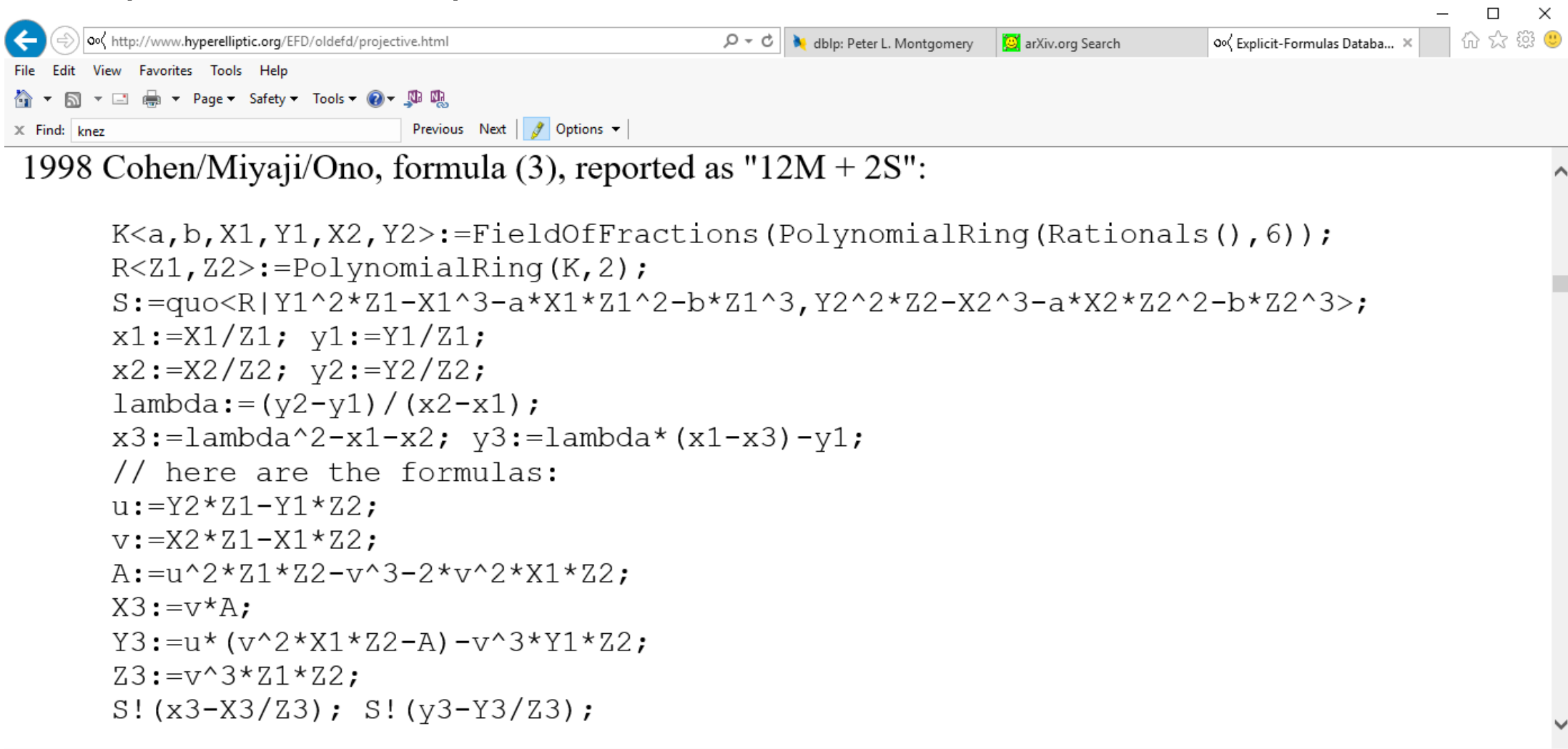
*: In practice, Shor's quantum algorithm scales as $O(n^3 \log n)$.

Basis for RSA/EC signature

A collage of images related to digital security and services, including a browser window showing Bank of America, credit cards (Maestro, VISA), OneDrive for Business, and SharePoint. There are also graphs with curves and a key icon.

Recent result: circuit for Shor's
[Roetteler, Naehrig, Svore, Lauter, arxiv: 1706.06752]

Example: ECC point addition



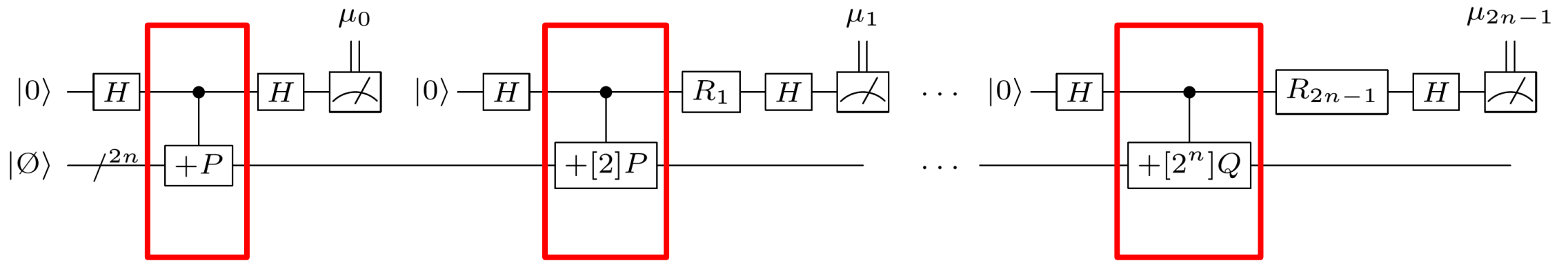
The screenshot shows a web browser window with the address bar containing `http://www.hyperelliptic.org/EFD/olddefd/projective.html`. The browser's menu bar includes File, Edit, View, Favorites, Tools, and Help. Below the menu bar is a search bar with the text "Find: knez". The main content area of the browser displays the following code:

```
1998 Cohen/Miyaji/Ono, formula (3), reported as "12M + 2S":  
  
K<a,b,X1,Y1,X2,Y2>:=FieldOfFractions(PolynomialRing(Rationals(),6));  
R<Z1,Z2>:=PolynomialRing(K,2);  
S:=quo<R|Y1^2*Z1-X1^3-a*X1*Z1^2-b*Z1^3,Y2^2*Z2-X2^3-a*X2*Z2^2-b*Z2^3>;  
x1:=X1/Z1; y1:=Y1/Z1;  
x2:=X2/Z2; y2:=Y2/Z2;  
lambda:=(y2-y1)/(x2-x1);  
x3:=lambda^2-x1-x2; y3:=lambda*(x1-x3)-y1;  
// here are the formulas:  
u:=Y2*Z1-Y1*Z2;  
v:=X2*Z1-X1*Z2;  
A:=u^2*Z1*Z2-v^3-2*v^2*X1*Z2;  
X3:=v*A;  
Y3:=u*(v^2*X1*Z2-A)-v^3*Y1*Z2;  
Z3:=v^3*Z1*Z2;  
S!(x3-X3/Z3); S!(y3-Y3/Z3);
```

[Bernstein, Lange: Database of explicit ECC formulas: <http://www.hyperelliptic.org/EFD/>]

High-level structure of the quantum algorithm

Phase estimation framework:



- Except for Hadamard H , rotations R_i and measurements, all gates in these circuits can be implemented over the Toffoli gate set.
- This allows to construct the circuit and simulate it on a classical machine.
- Precise resource estimates can be obtained from reference implementation.

Montgomery inversion

Algorithm MONTINVERSE

Inputs: a, b, n , where a is odd, $a > b > 0$, and n is the number of bits in a

Output: “Not relatively prime,” or $b^{-1}2^n \bmod a$

First phase

$u \leftarrow a, v \leftarrow b, r \leftarrow 0, s \leftarrow 1$

$k \leftarrow 0$

while $v > 0$ **do**

if u is even **then** $u \leftarrow u/2, s \leftarrow 2s$

else if v is even **then** $v \leftarrow v/2, r \leftarrow 2r$

else if $u > v$ **then** $u \leftarrow (u - v)/2, r \leftarrow r + s, s \leftarrow 2s$

else $v \leftarrow (v - u)/2, s \leftarrow r + s, r \leftarrow 2r$

$k \leftarrow k + 1$

if $u \neq 1$ **then return** “Not relatively prime”

if $r \geq a$ **then** $r \leftarrow r - a$

Second phase

for $i \leftarrow 1$ **to** $k - n$ **do**

if r is even **then** $r \leftarrow r/2$

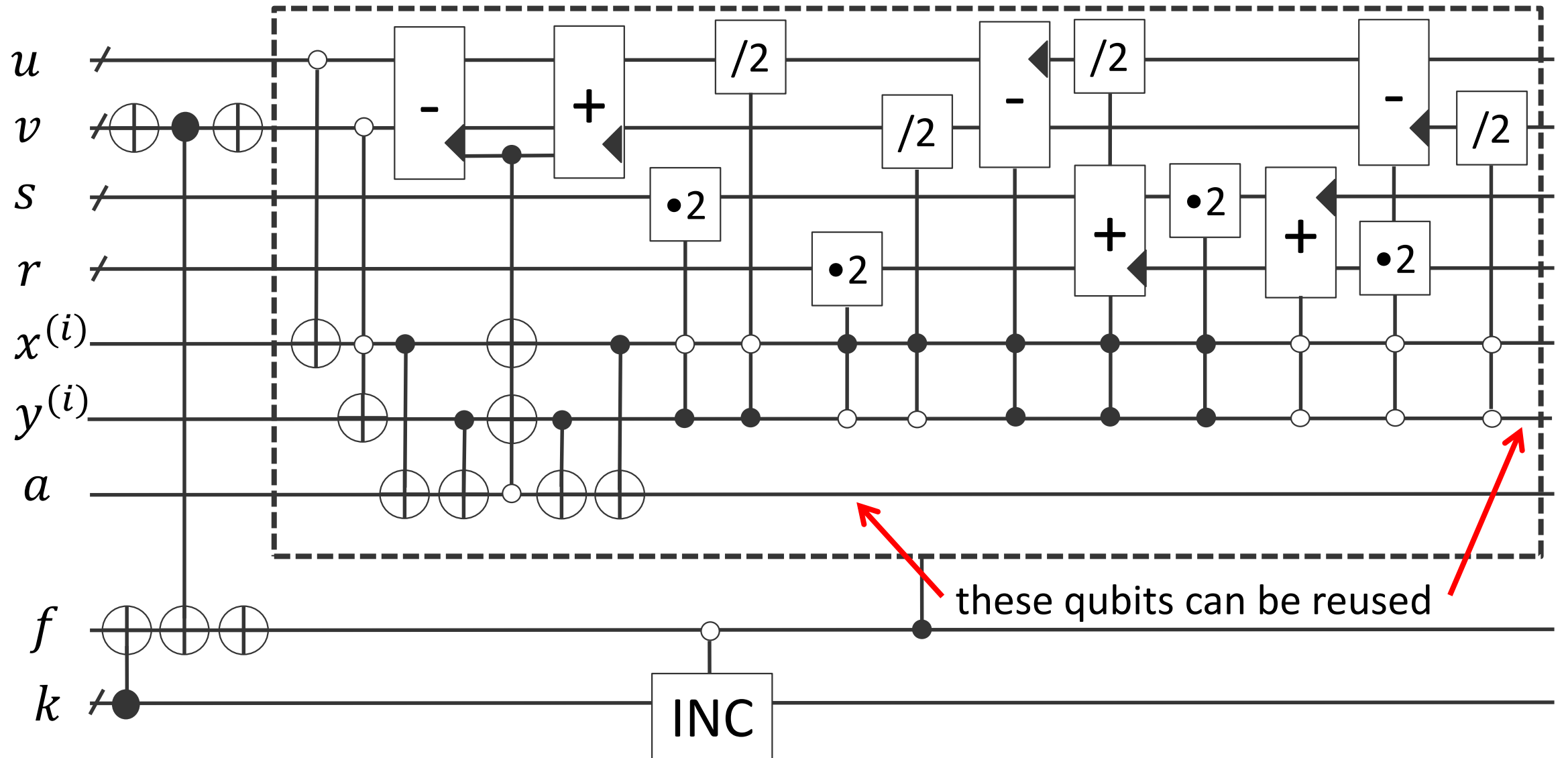
else $r \leftarrow (r + a)/2$

return $a - r$

- Requires to handle a WHILE loop (with known upper bound (here: $2n$))
- Implemented in LIQUi|>, including P-192, P-224, P-256, P-384, P-521

[B. Kaliski, IEEE Trans. Comp. 44(8), 1995]

Quantum Montgomery arithmetic



Quantum circuits to attack ECC dlog

Implementing point addition: affine Weierstrass form

```

1: sub_const_modp  $x_1$   $x_2$ ; //  $x_1 \leftarrow x_1 - x_2$ 
2: ctrl_sub_const_modp  $y_1$   $y_2$  ctrl; //  $y_1 \leftarrow [y_1 - y_2]_1, [y_1]_0$ 
3: inv_modp  $x_1$   $t_0$ ;
4: mul_modp  $y_1$   $t_0$   $\lambda$ ;
5: mul_modp  $\lambda$   $x_1$   $y_1$ ;
6: inv_modp  $x_1$   $t_0$ ;
7: squ_modp  $\lambda$   $t_0$ ;
8: ctrl_sub_modp  $x_1$ 
9: ctrl_add_const_m
10: squ_modp  $\lambda$   $t_0$ ;
11: mul_modp  $\lambda$   $x_1$   $y_1$ ;
12: inv_modp  $x_1$   $t_0$ ;
13: mul_modp  $t_0$   $y_1$   $\lambda$ ;
14: inv_modp  $x_1$   $t_0$ ;
15: ctrl_neg_modp  $x_1$ 
16: ctrl_sub_const_m
17: add_const_modp  $x$ 

```

Modular arithmetic circuit	# of qubits		# Toffoli gates
	total	ancillas	
add_const_modp, sub_const_modp	$2n$	n	$16n \log_2(n) - 26.9n$
ctrl_add_const_modp, ctrl_sub_const_modp	$2n + 1$	n	$16n \log_2(n) - 26.9n$
ctrl_sub_modp	$2n + 4$	3	$16n \log_2(n) - 23.8n$
ctrl_neg_modp	$n + 3$	2	$8n \log_2(n) - 14.5n$
mul_modp (dbl/add)	$3n + 2$	2	$32n^2 \log_2(n) - 59.4n^2$
mul_modp (Montgomery)	$5n + 4$	$2n + 4$	$16n^2 \log_2(n) - 26.3n^2$
squ_modp (dbl/add)	$2n + 3$	3	$32n^2 \log_2(n) - 59.4n^2$
squ_modp (Montgomery)	$4n + 5$	$2n + 5$	$16n^2 \log_2(n) - 26.3n^2$
inv_modp	$7n + 2\lceil \log_2(n) \rceil + 9$	$5n + 2\lceil \log_2(n) \rceil + 9$	$32n^2 \log_2(n)$

Comparing quantum attacks

ECDLP in $E(\mathbb{F}_p)$ simulation results					Factoring of RSA modulus N interpolation from [18]		
$\lceil \log_2(p) \rceil$ bits	#Qubits	#Toffoli gates	Toffoli depth	Sim time sec	$\lceil \log_2(N) \rceil$ bits	#Qubits	#Toffoli gates
110	1014	$9.44 \cdot 10^9$	$8.66 \cdot 10^9$	273	512	1026	$6.41 \cdot 10^{10}$
160	1466	$2.97 \cdot 10^{10}$	$2.73 \cdot 10^9$	711	1024	2050	$5.81 \cdot 10^{11}$
192	1754	$5.30 \cdot 10^{10}$	$4.86 \cdot 10^{10}$	1 149	—	—	—
224	2042	$8.43 \cdot 10^{10}$	$7.73 \cdot 10^{10}$	1 881	2048	4098	$5.20 \cdot 10^{12}$
256	2330	$1.26 \cdot 10^{11}$	$1.16 \cdot 10^{11}$	3 848	3072	6146	$1.86 \cdot 10^{13}$
384	3484	$4.52 \cdot 10^{11}$	$4.15 \cdot 10^{11}$	17 003	7680	15362	$3.30 \cdot 10^{14}$
521	4719	$1.14 \cdot 10^{12}$	$1.05 \cdot 10^{12}$	42 888	15360	30722	$2.87 \cdot 10^{15}$

- Our implementation of ECC dlog (ECDLP) for size n scales as $448n^3 \log_2 n + O(n^3)$ Toffoli gates and $9n + \lceil \log_2 n \rceil + 10$ qubits. For RSA the scaling is $64n^3 \log_2 n + O(n^3)$ and $2n + 2$ qubits.
- Timings with respect to LIQUII) running on HP ProLiant DL580 (4 Xeons @ 2.30GHz and 3TB memory)
- For example, bit size $n = 256$ corresponds to ECDLP used in bitcoin curve `secp256k1`
- Confirms estimates by Proos & Zalka and implies that ECDLP is easier quantum target than RSA.

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