

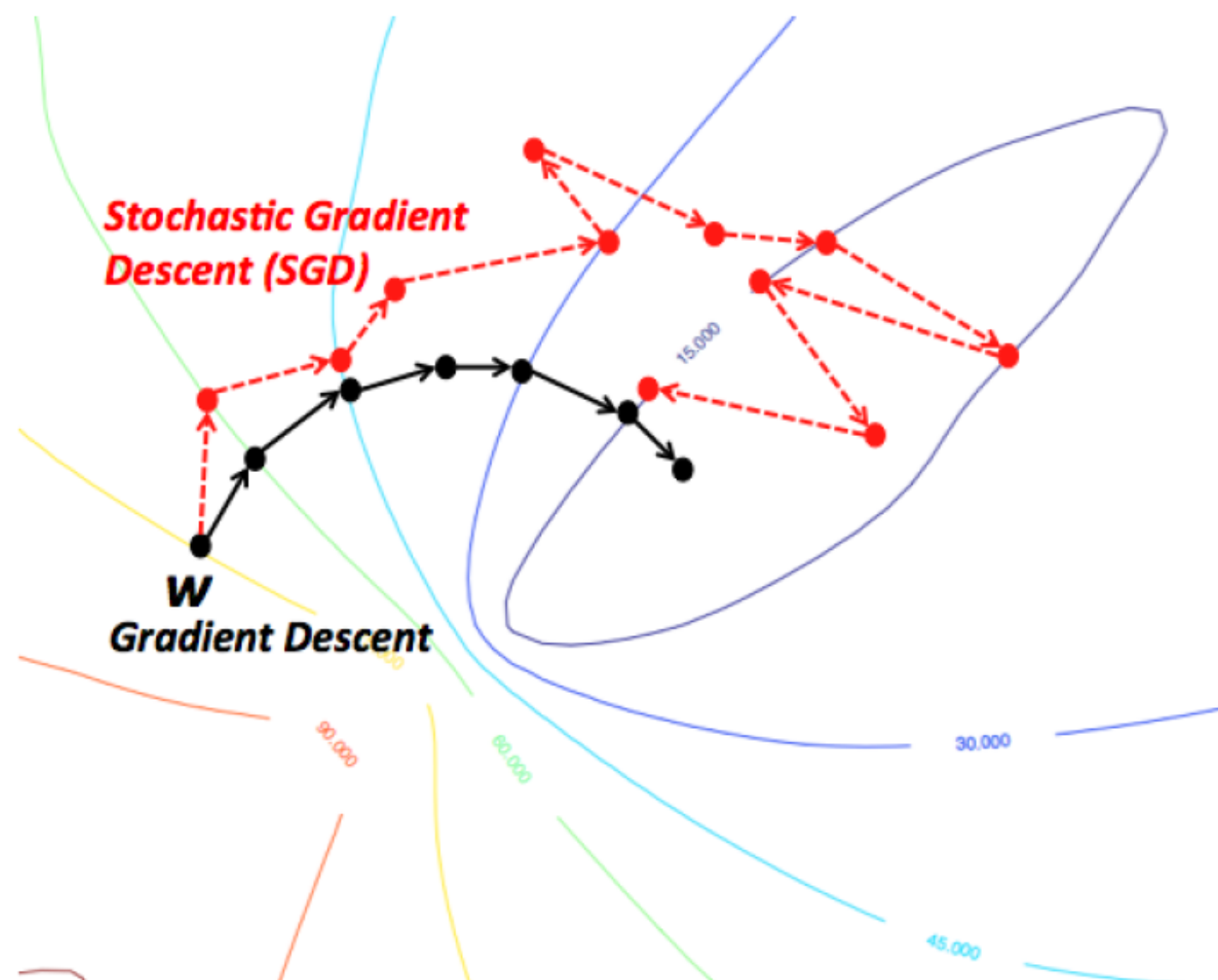
# Estimating gradients using quantum computation and Forest

Rigetti quantum computing meetup  
November 2, 2017

Keri A. McKiernan  
[kmckiern.github.io](https://github.com/kmckiern)

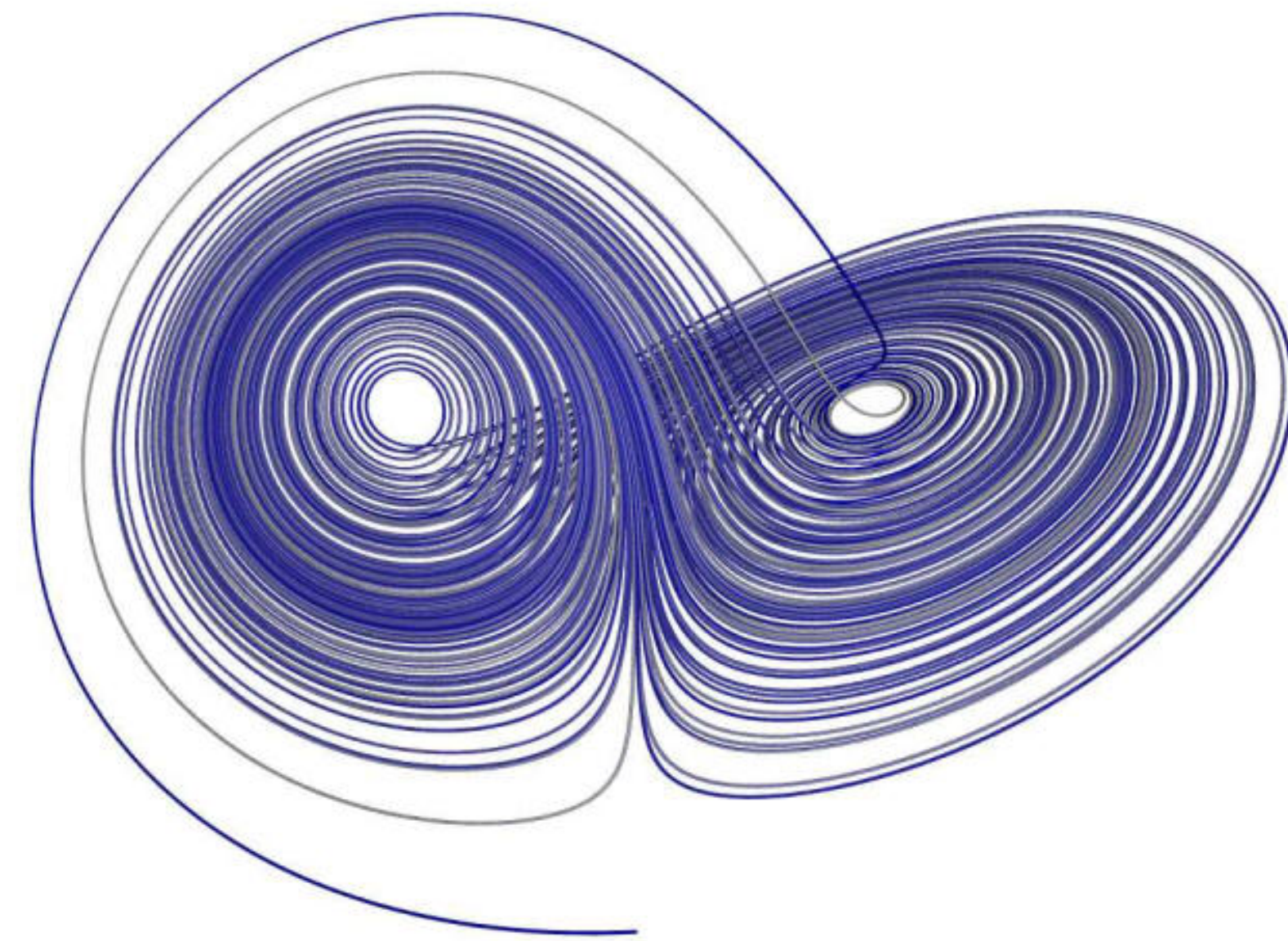
# Gradients are fundamental to research and engineering applications

Optimization problems



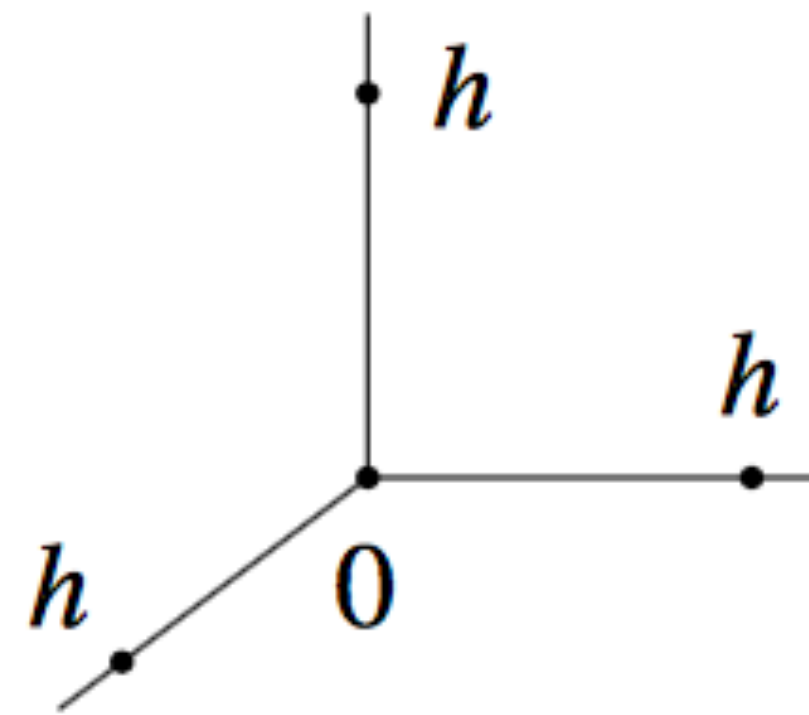
<https://wikidocs.net/3413>

Dynamical systems

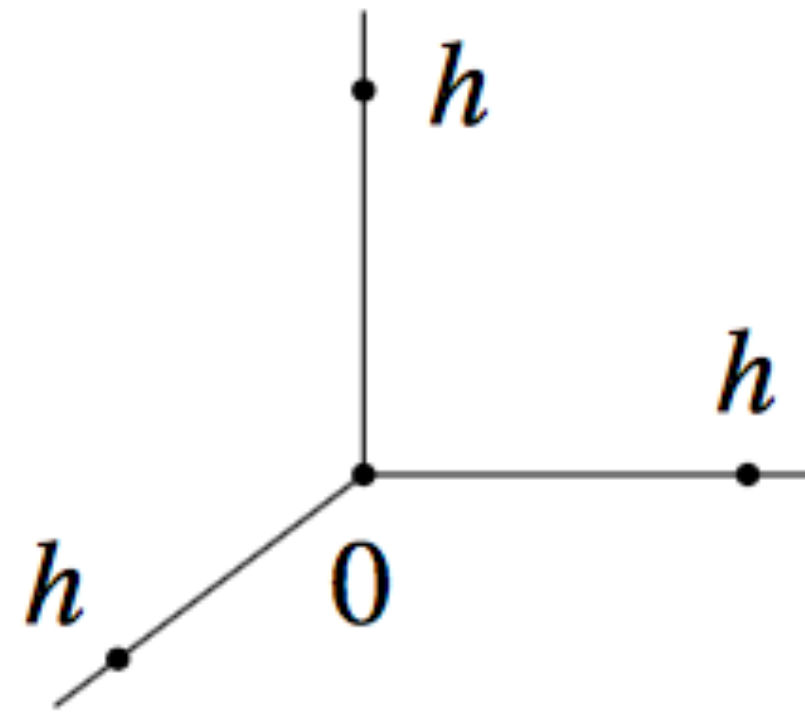


<https://www.math.uci.edu/~asgor/dynsys/>

# Computing numerical gradient estimates

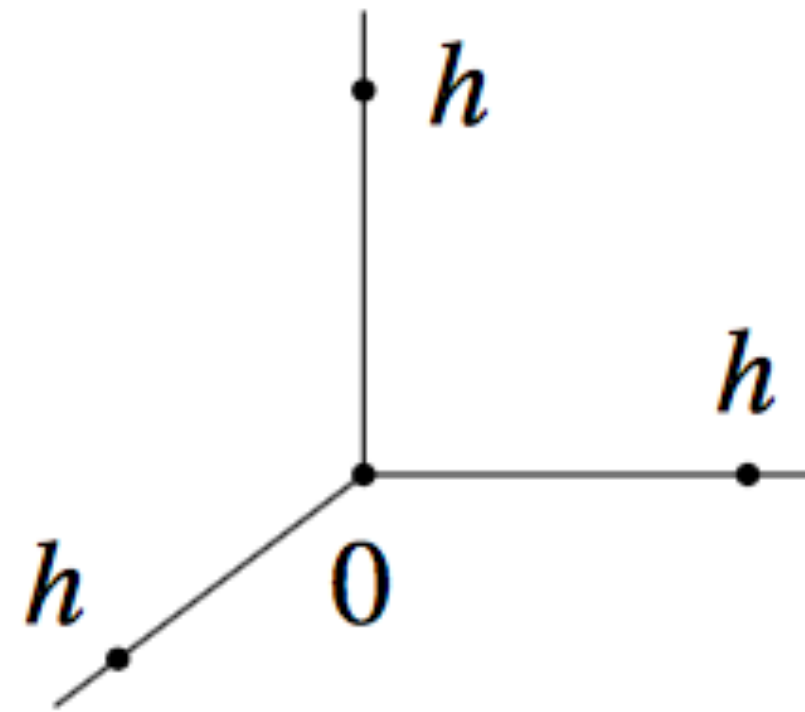


# Computing numerical gradient estimates



$$E(h) \approx E(0) + h \nabla E(0)$$

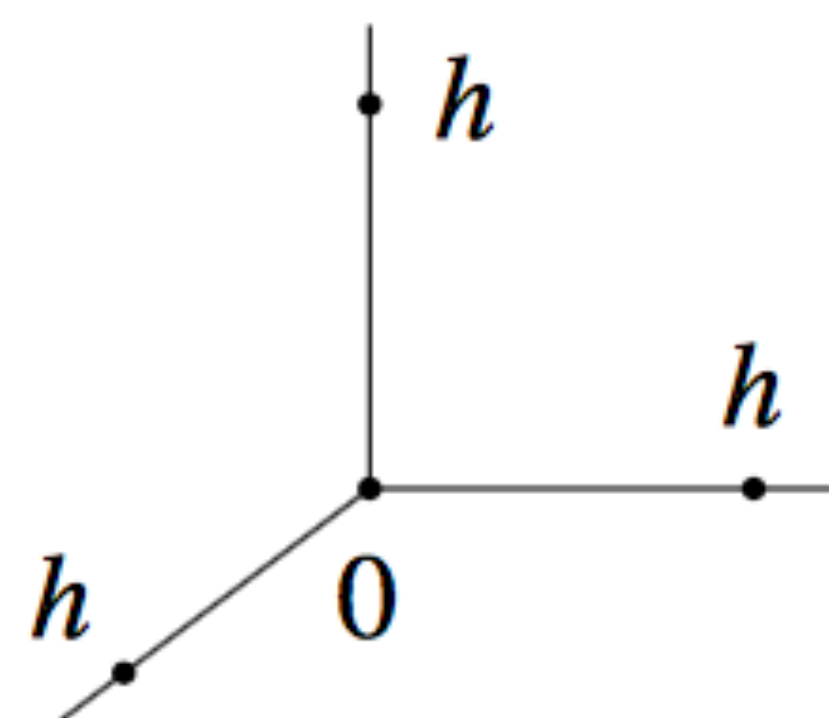
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$$\nabla E(0) \approx \frac{E(0) - E(h)}{h}$$

# Numerical gradient estimation is fast on quantum architecture



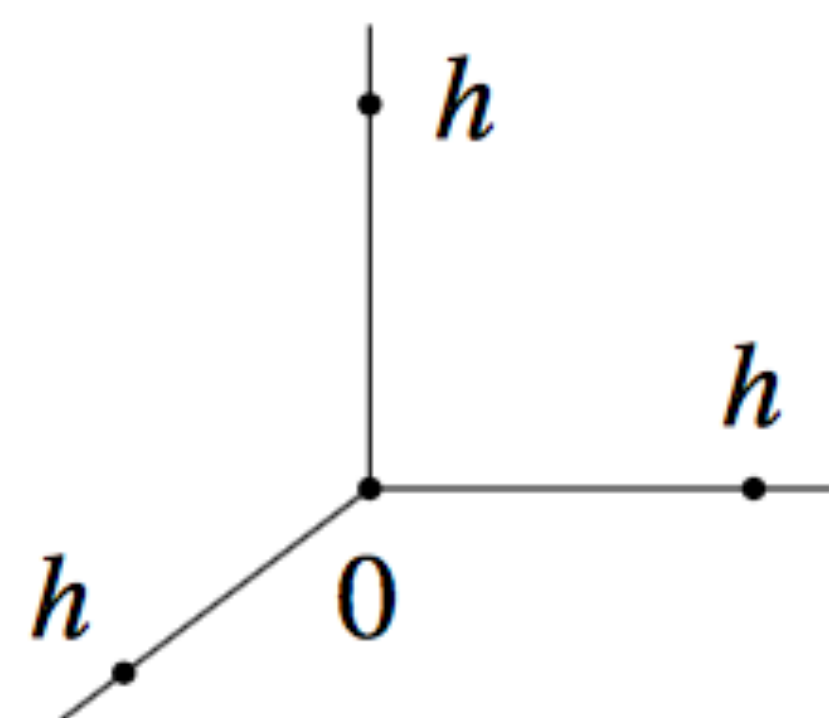
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	Classical		Quantum
Derivative	Numerical	Analytical	Numerical
$\frac{dE}{d\mu}$	$d + 1$	$O(1)$	1
$\frac{d^2 E}{d\mu^2}$	$d^2 + 1$	$O(d)$	2
$\frac{d^3 E}{d\mu^3}$	$d^3 + 1$	$O(d)$	4
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\frac{d^n E}{d\mu^n}$	$d^n + 1$	$O\left(d^{\lfloor n/2 \rfloor}\right)$	$2^{n-1}$



# Numerical gradient estimation is fast on quantum architecture

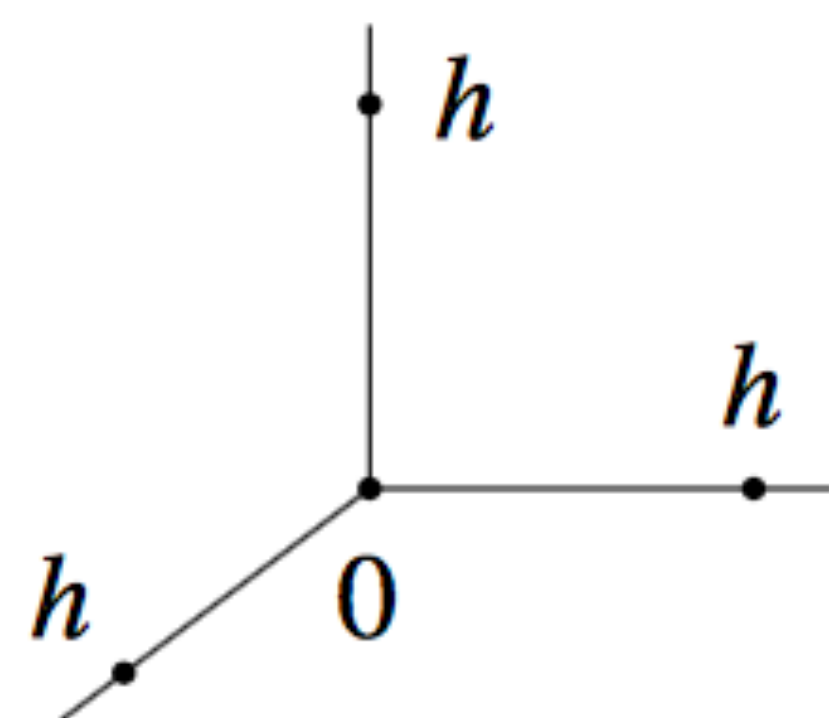


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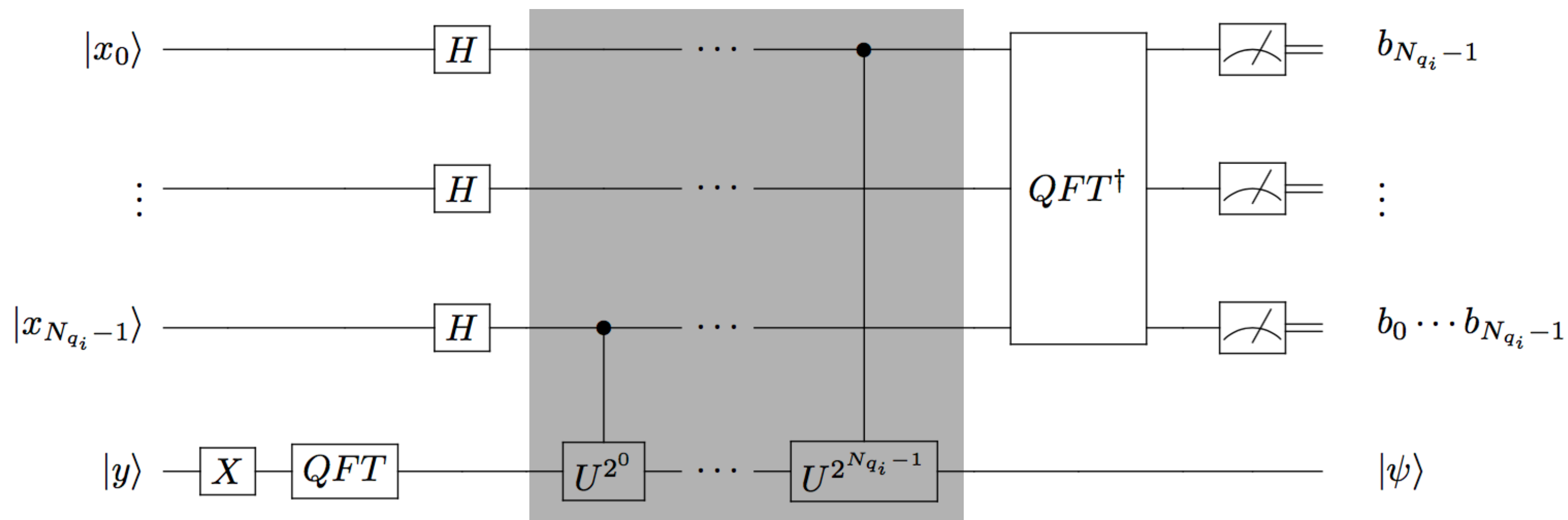
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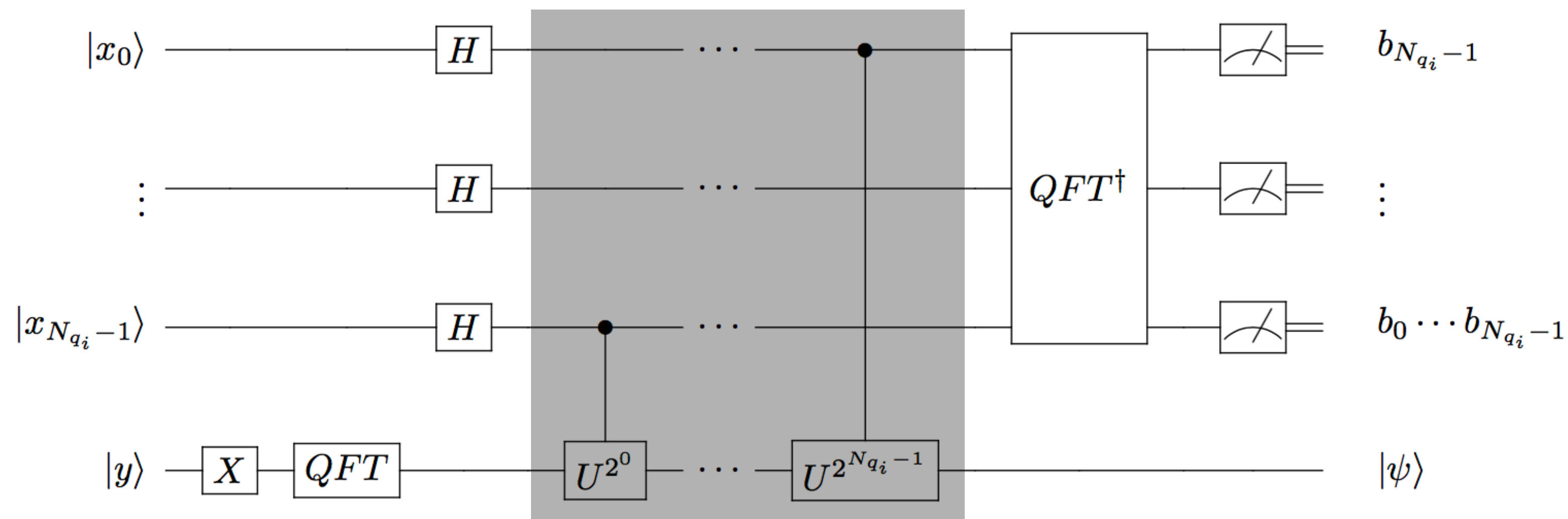
# Jordan gradient estimation

$$f : \mathbb{R}^d \rightarrow \mathbb{R}$$

$$\vec{\nabla} f(\vec{x}) \approx 0.b_0 \cdots b_{n-1}$$

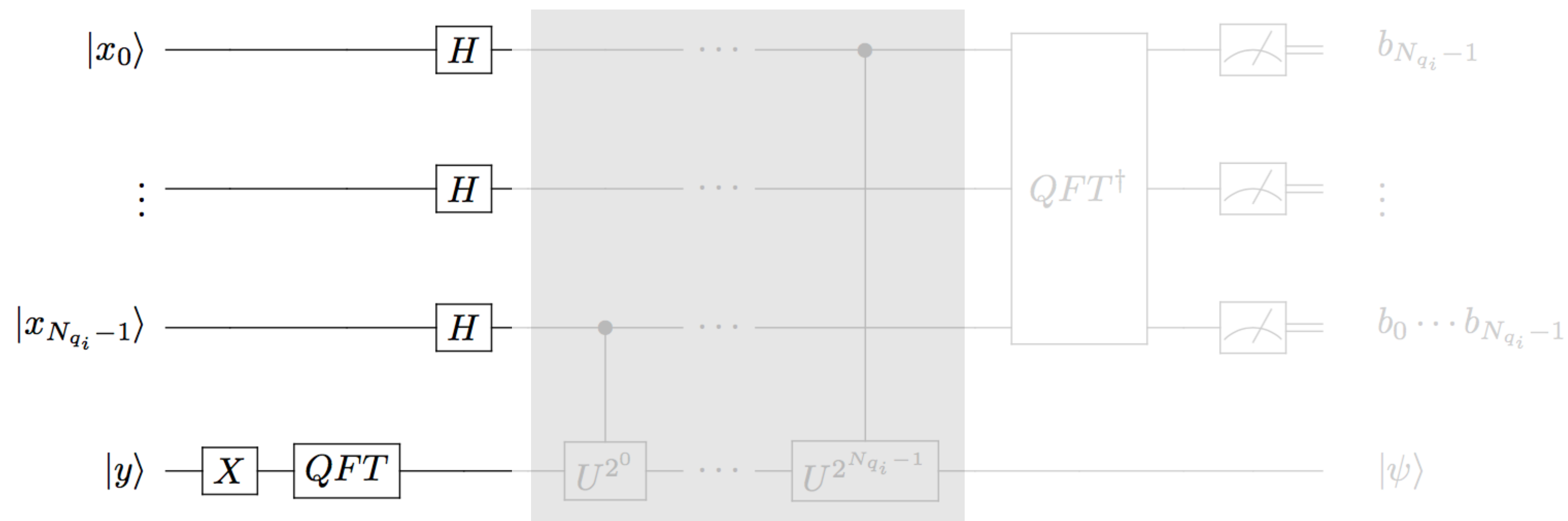


# Jordan gradient estimation



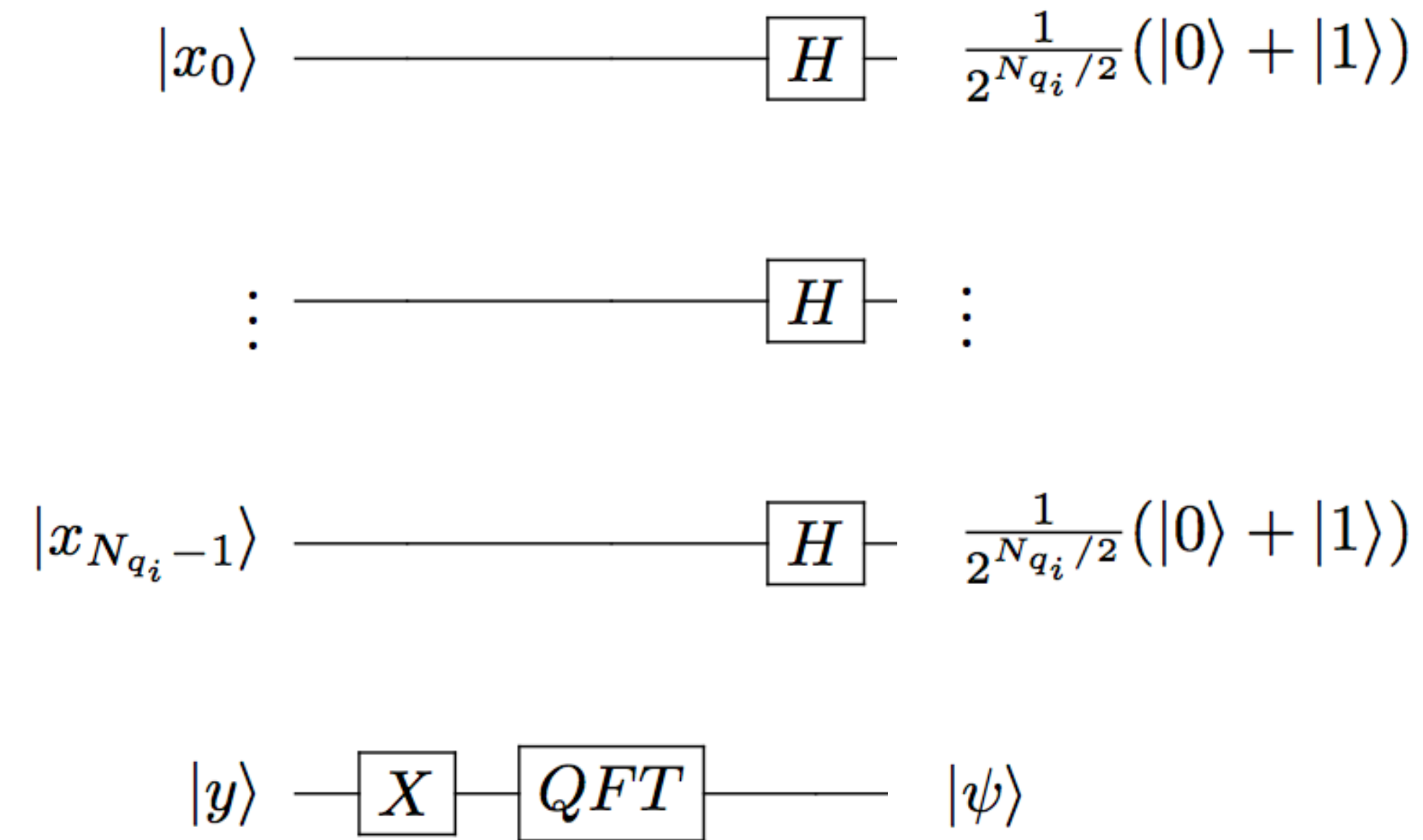
program	ancilla qubits	input qubits
initialize system	QFT, X	H
phase kickback	U	IQFT
measure	-	M

# Jordan gradient estimation



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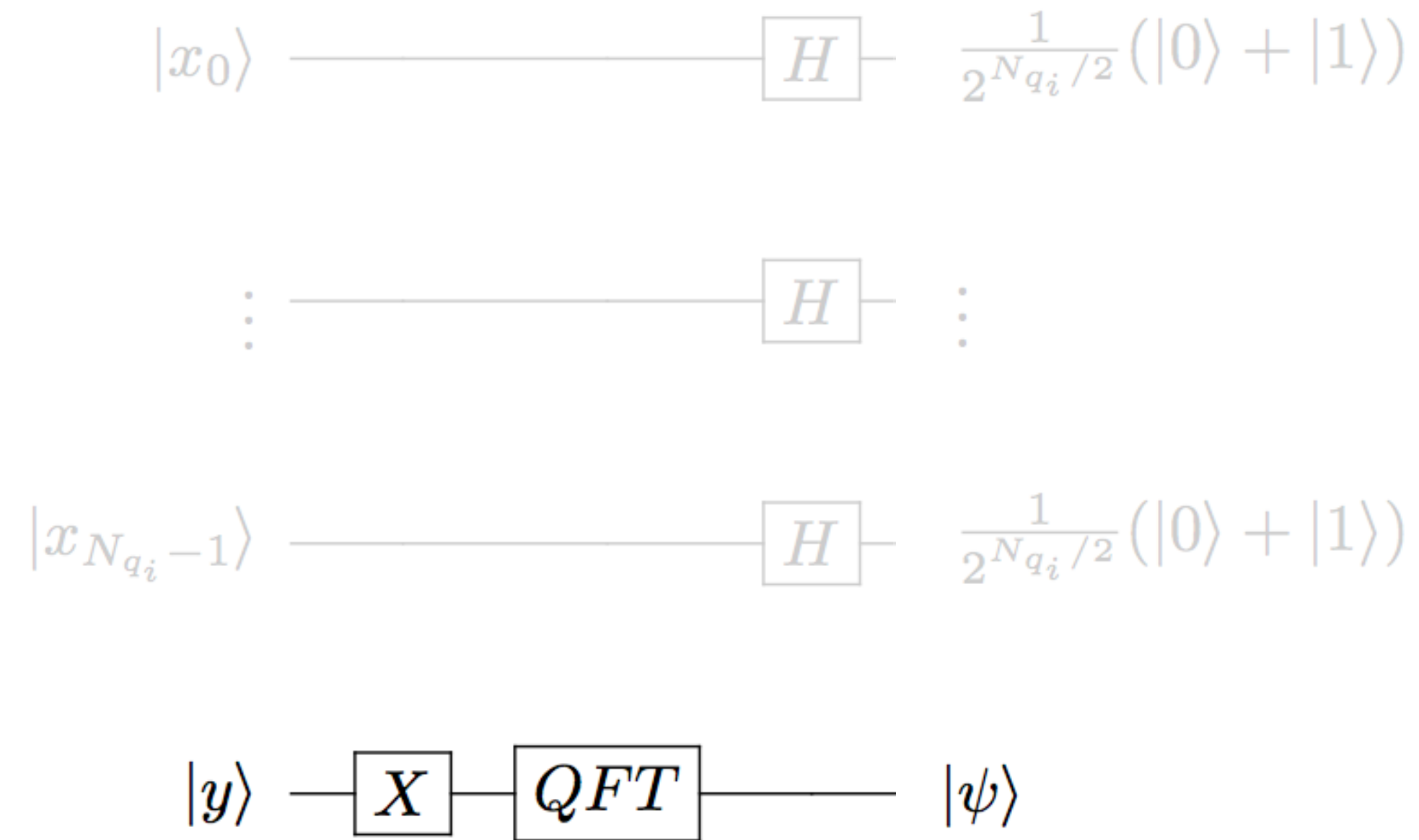
# initialize system



Prepare the ancilla register to a plane wave state

$$|\psi\rangle = \frac{1}{\sqrt{2^{N_{q_o}}}} \sum_{k=0}^{2^{N_{q_o}}-1} e^{i2\pi k/2^{N_{q_o}}} |k\rangle \quad (1)$$

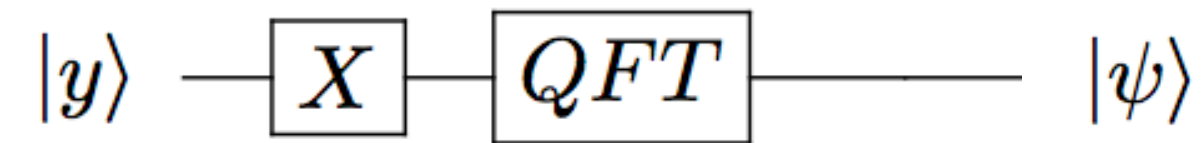
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# initialize system



```
from pyquil.gates import X
from grove.qft.fourier import qft
import pyquil.quil as pq

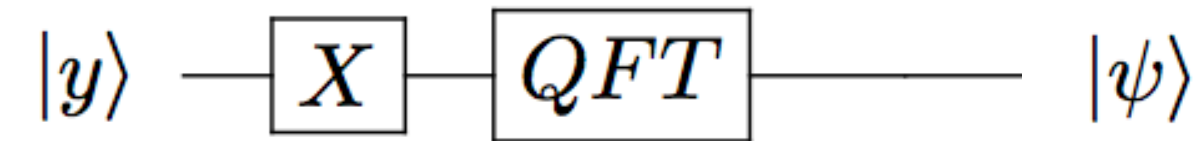
def initialize_system(input_qubits, ancilla_qubits):
    """ Prepare initial state

    :param list input_qubit: Qubits of input registers.
    :param list ancilla_qubits: Qubits of output register.
    :return Program p_ic: Quil program to initialize this system.
    """

    # ancilla qubits to plane wave state
    ic_out = list(map(X, ancilla_qubits))
    ft_out = qft(ancilla_qubits)
    p_ic_out = pq.Program(ic_out) + ft_out
    # input qubits to equal superposition
    ic_in = list(map(H, input_qubits))
    p_ic_in = pq.Program(ic_in)
    # combine programs
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```



# initialize system



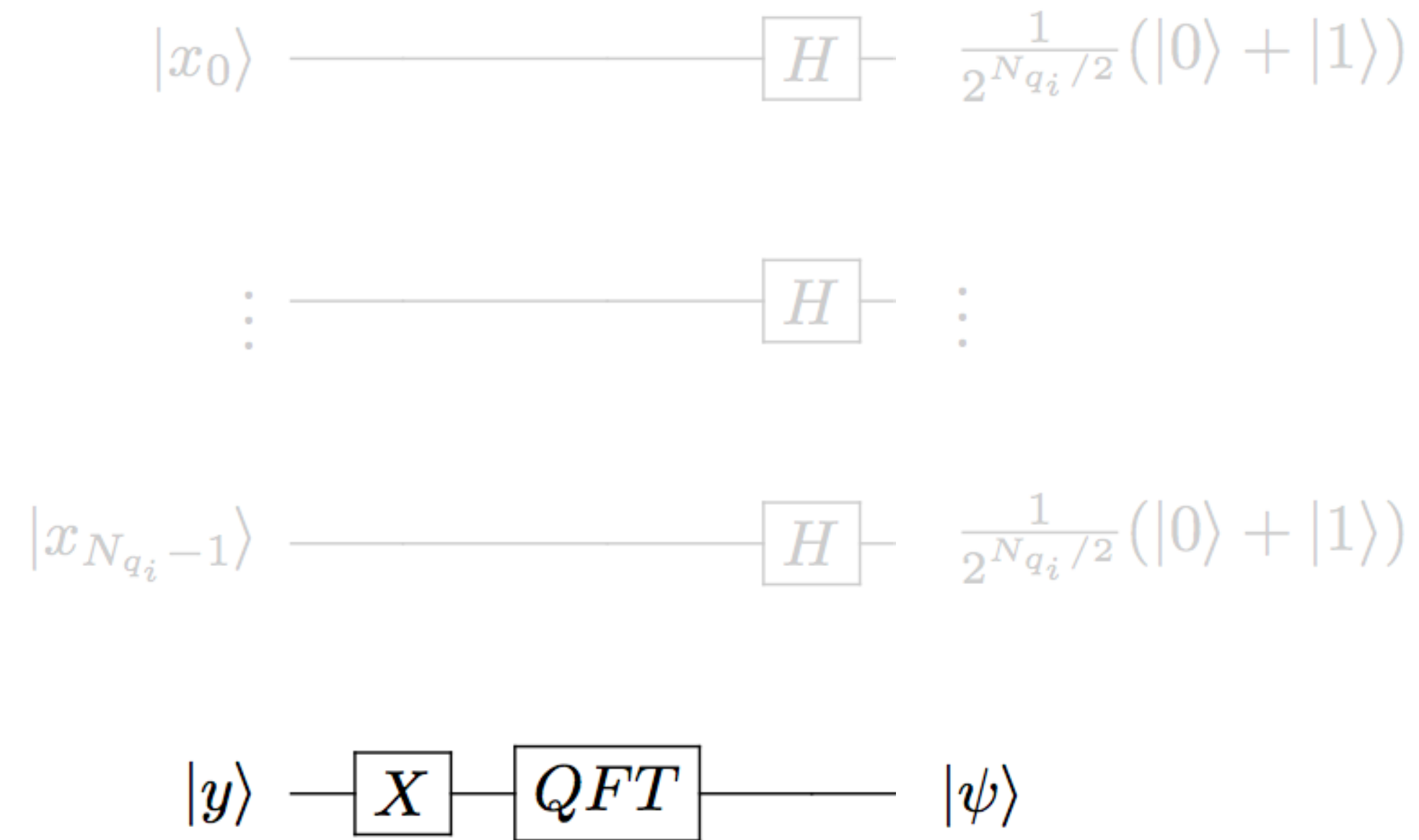
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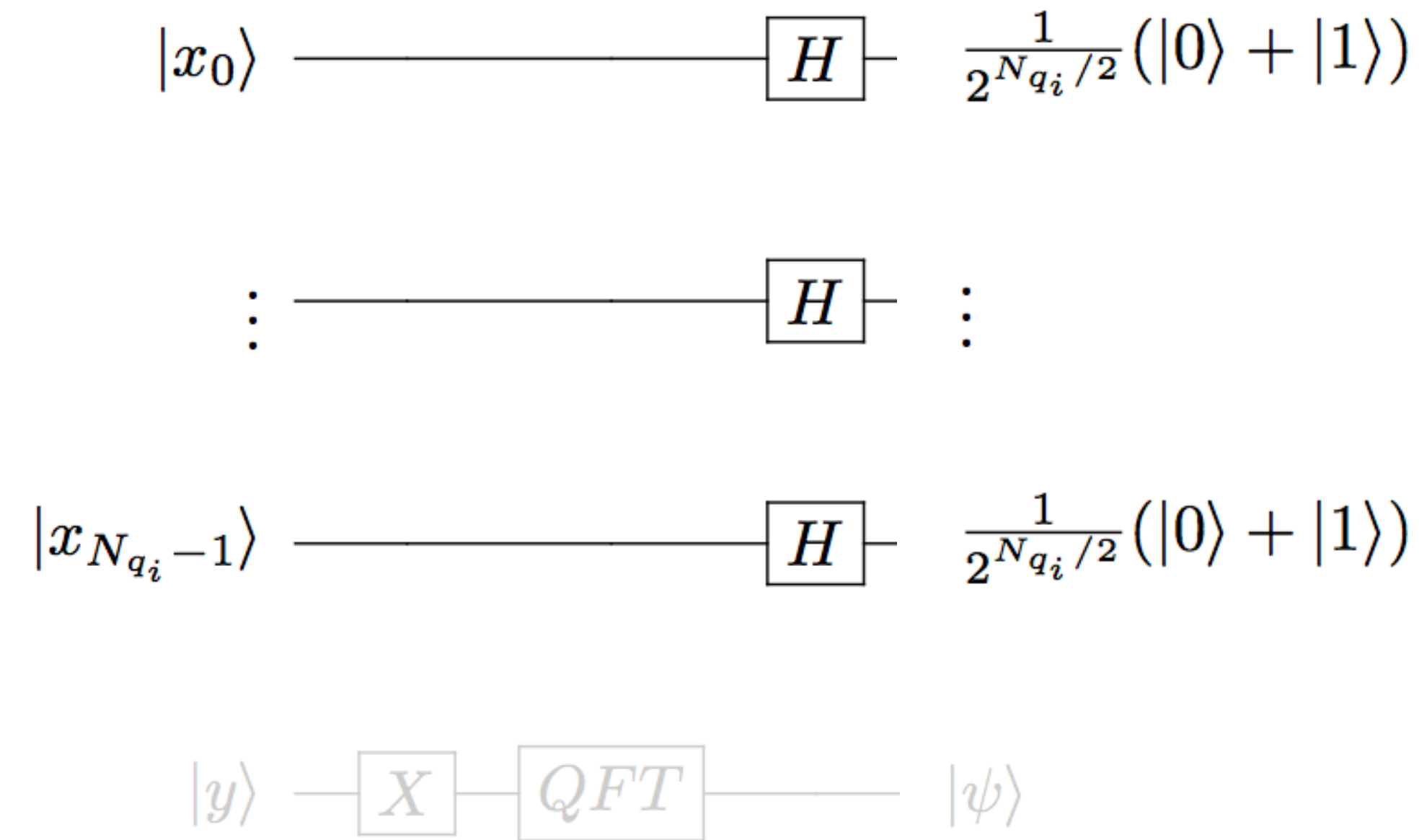
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$$\begin{array}{ccc} |x_0\rangle & \text{---} & \boxed{H} \text{---} \frac{1}{2^{N_{q_i}/2}} (|0\rangle + |1\rangle) \\ & & \\ \vdots & \text{---} & \boxed{H} \text{---} \vdots \\ & & \\ |x_{N_{q_i}-1}\rangle & \text{---} & \boxed{H} \text{---} \frac{1}{2^{N_{q_i}/2}} (|0\rangle + |1\rangle) \end{array}$$

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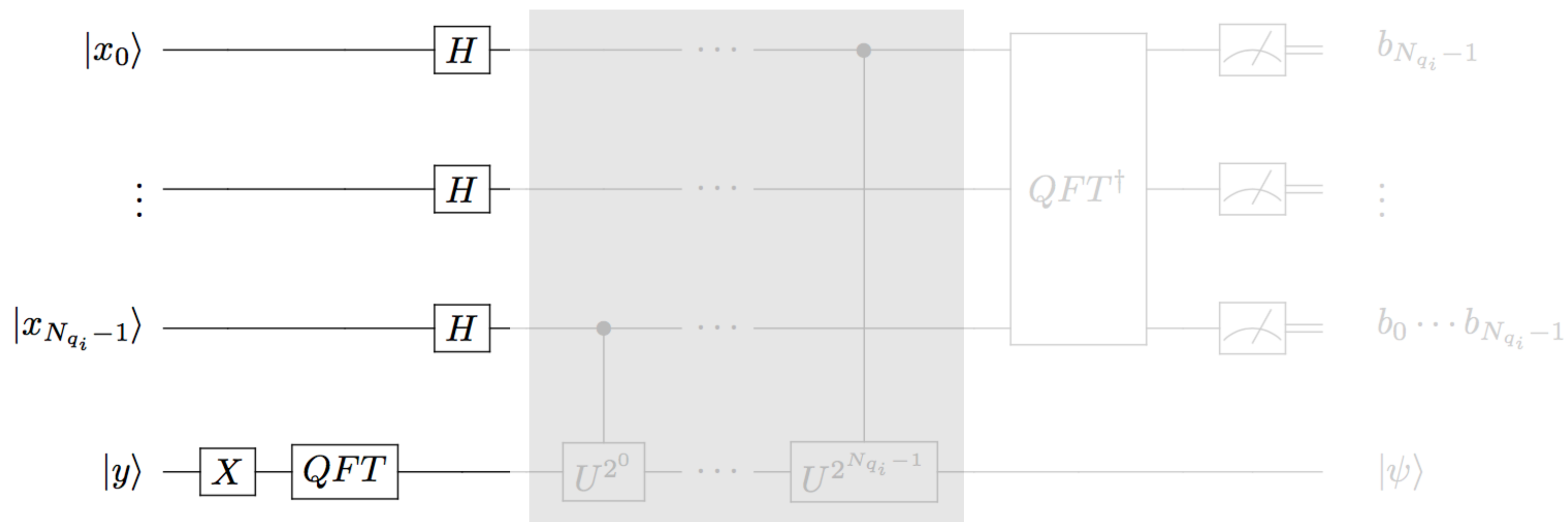
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program	ancilla qubits	input qubits
initialize system	QFT, X	H

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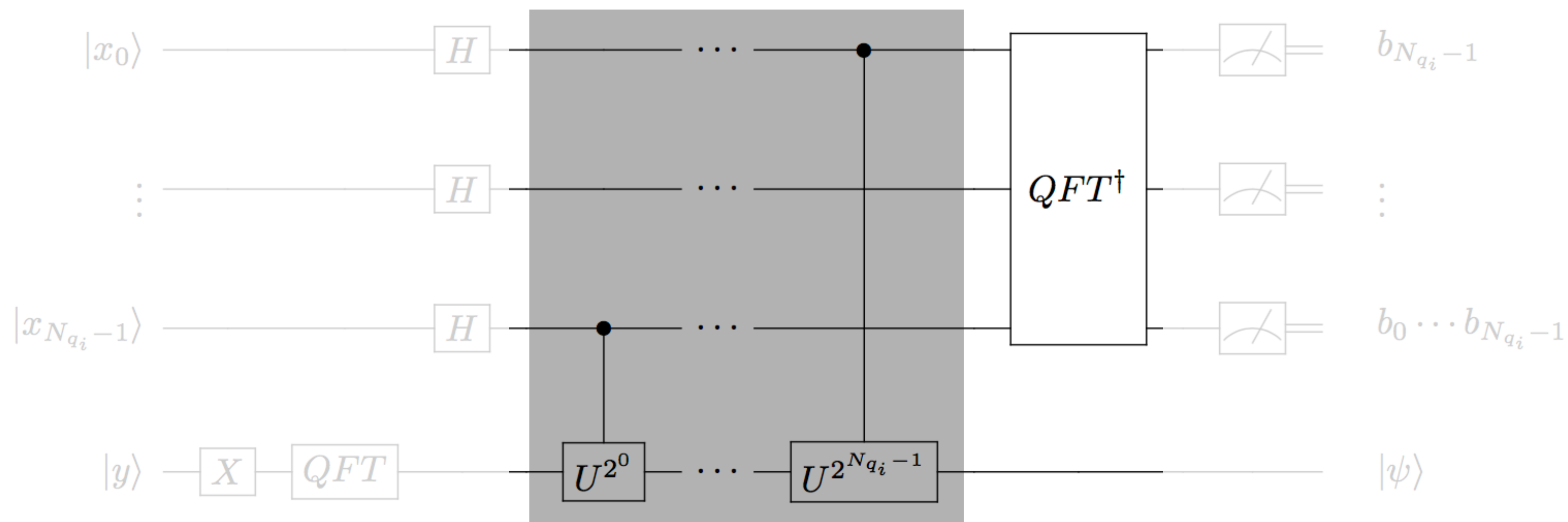


# Jordan gradient estimation



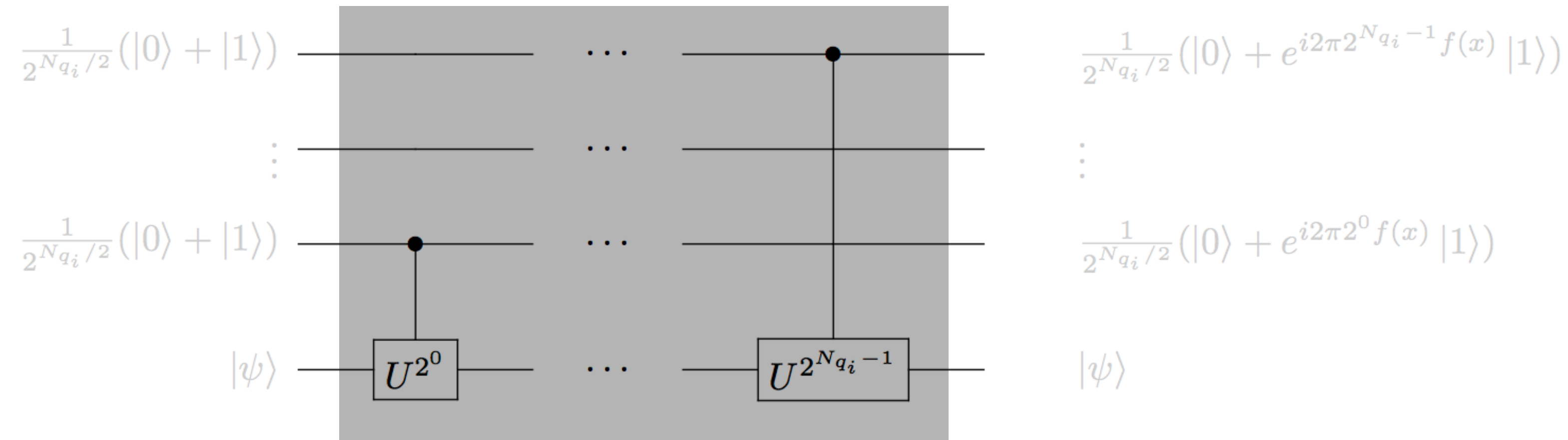
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# Jordan gradient estimation



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# phase kickback



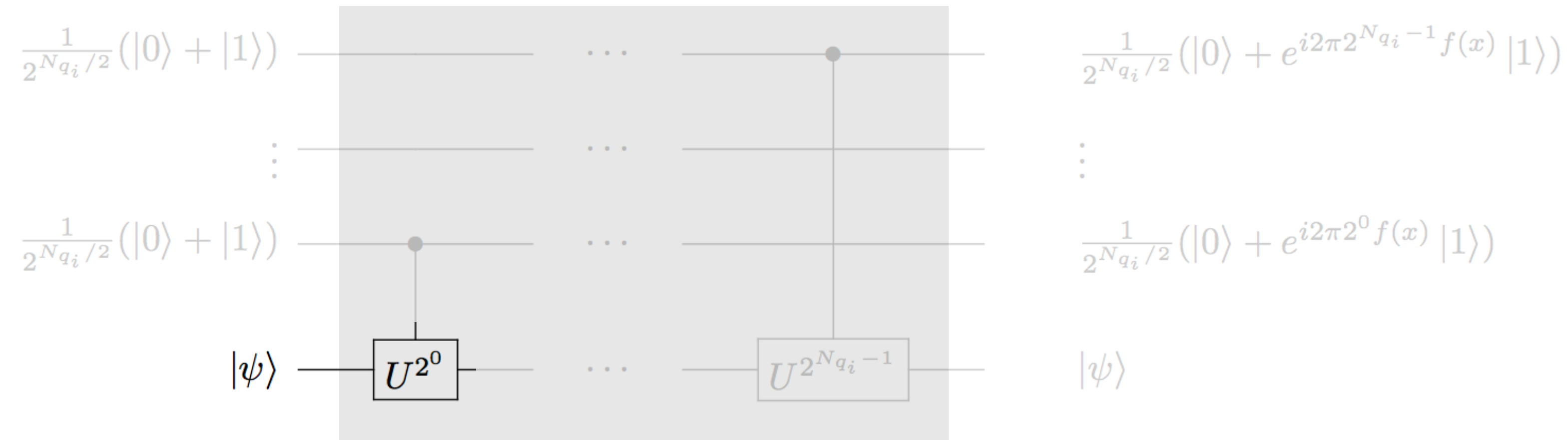
Construct  $U$  such that

$$U^{2^j} |\psi\rangle = e^{i2\pi 2^j f(x)} |\psi\rangle \quad (2)$$

Hence, we may use the PHASE gate for  $U$

$$U_{2\pi f(x)}^{2^j} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i2\pi 2^j f(x)} \end{bmatrix} \quad (3)$$

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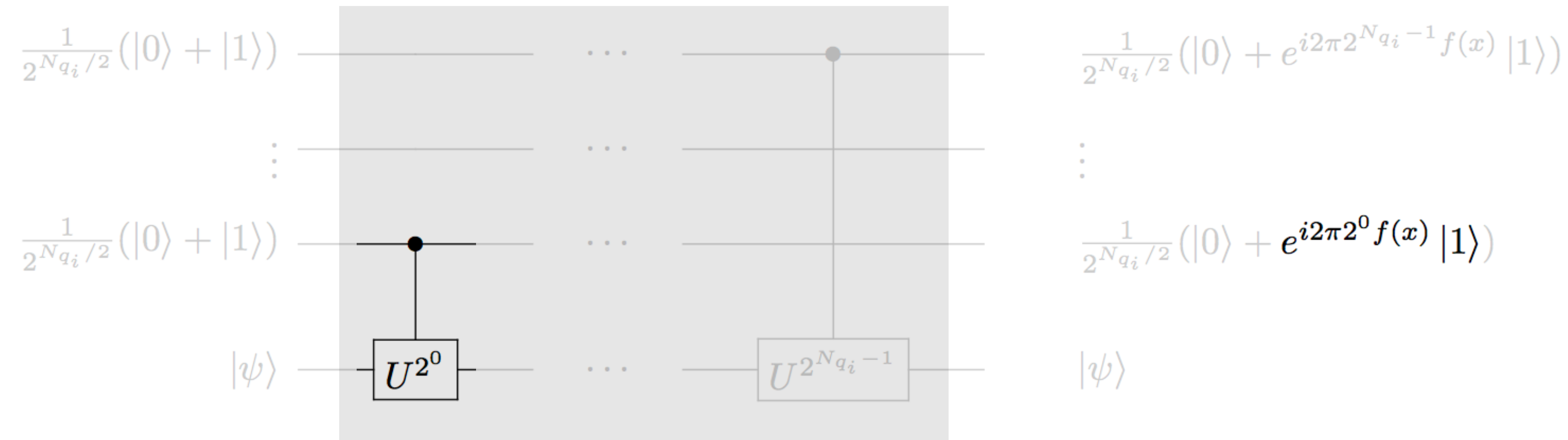
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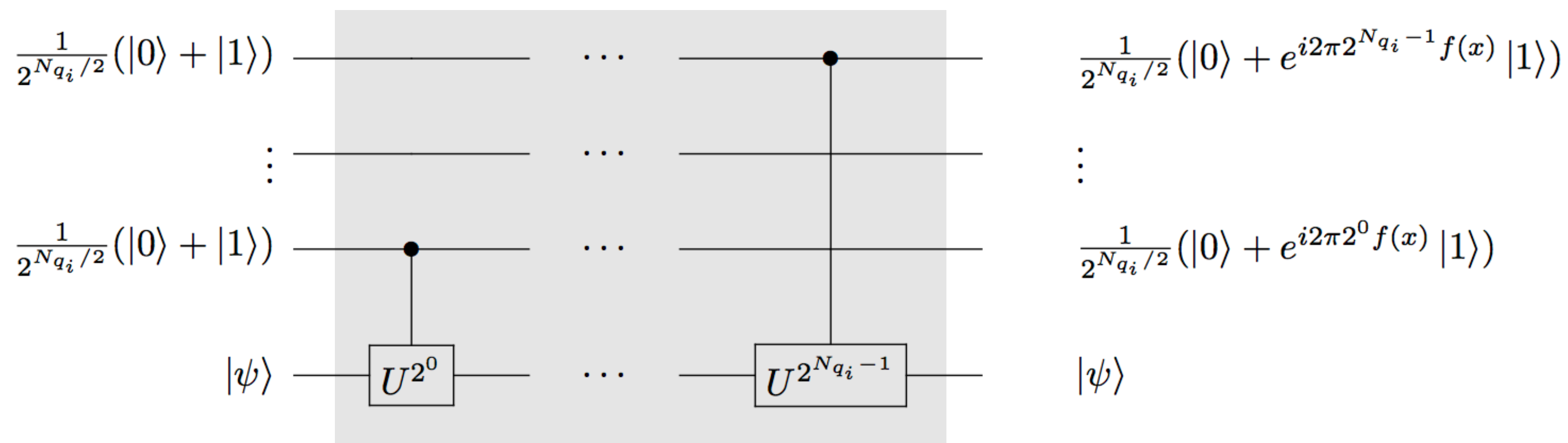
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from grove.alpha.phaseestimation.phase_estimation import controlled
from grove.qft.fourier import inverse_qft

# encode f_h into CPHASE gate
U = np.array([[1, 0],
              [0, np.exp(1.0j * np.pi * f_h)]])
p_kickback = pq.Program()
# apply c-U^{2^j} to ancilla register
for i in input_qubits:
    if i > 0:
        U = np.dot(U, U)
        cU = controlled(U)
        name = "c-U{0}".format(2 ** i)
        p_kickback.defgate(name, cU)
        p_kickback.inst((name, i, ancilla_qubits[0]))
# iqft to pull out fractional component of eigenphase
p_kickback += inverse_qft(input_qubits)
return p_kickback
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# phase kickback

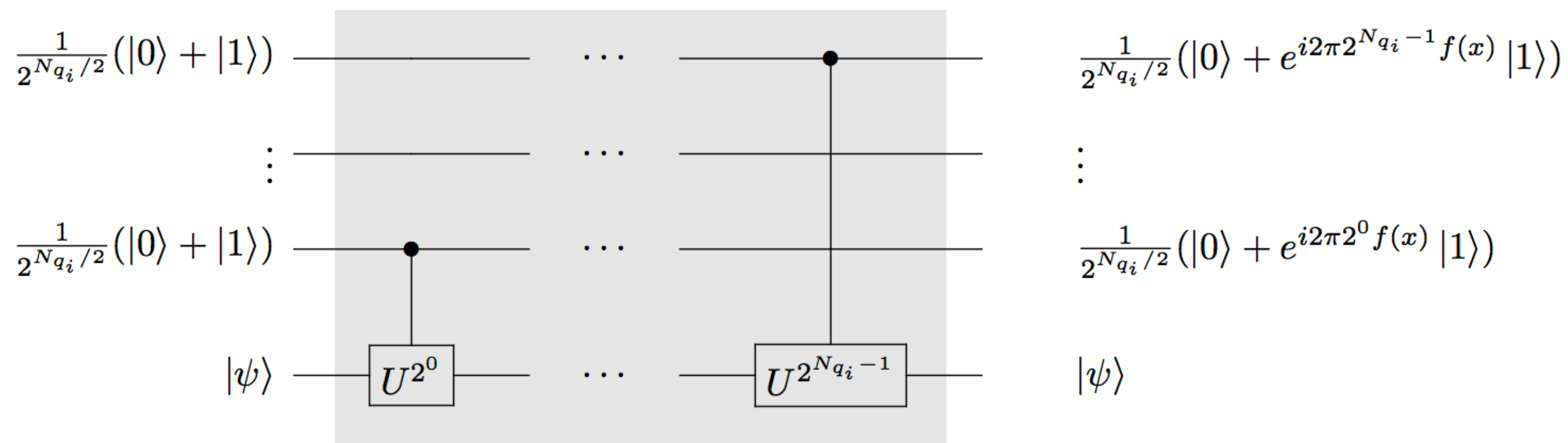
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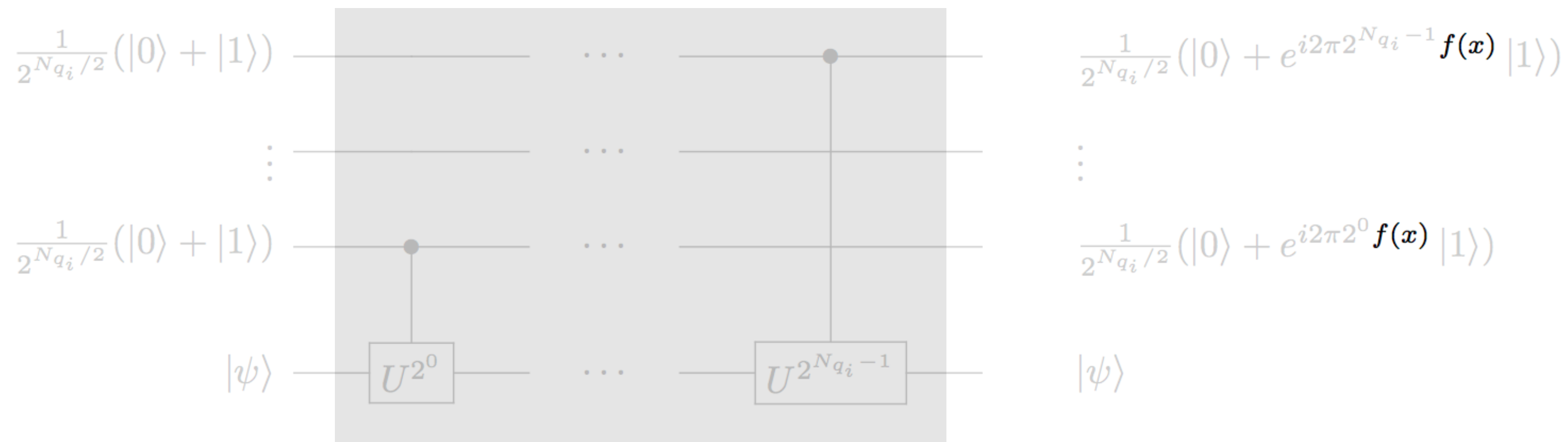
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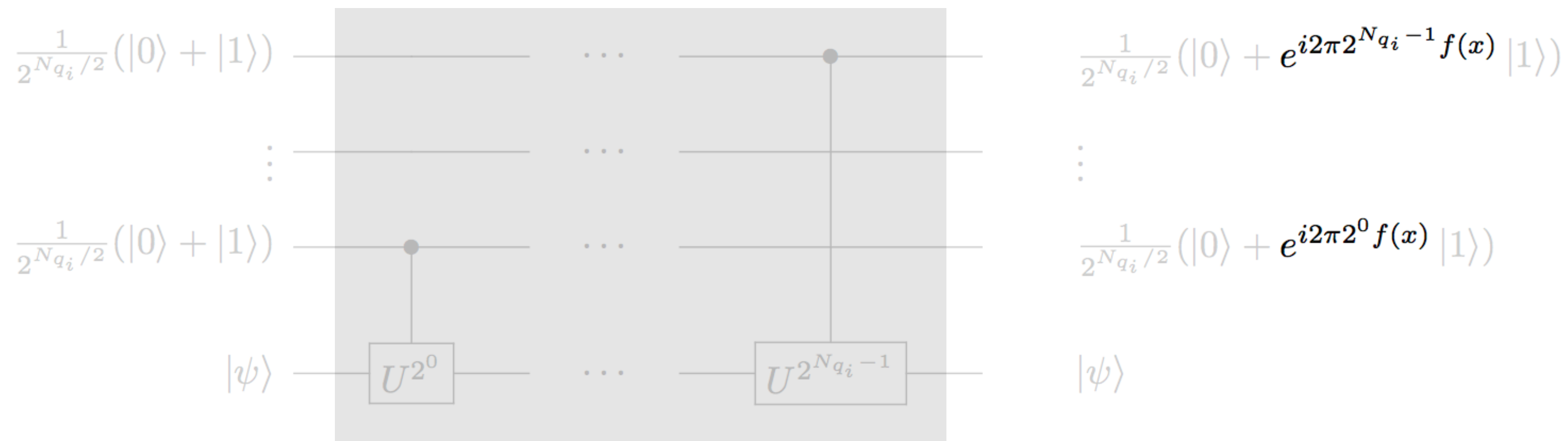
Sample  $f(h)$ . For small  $h$ , recall

$$f(h) \approx f(0) + h \nabla f(0) \quad (4)$$

So

$$e^{i2\pi 2^j f(h)} \approx e^{i2\pi 2^j f(0)} e^{i2\pi 2^j h \nabla f(0)} \quad (5)$$

# phase kickback



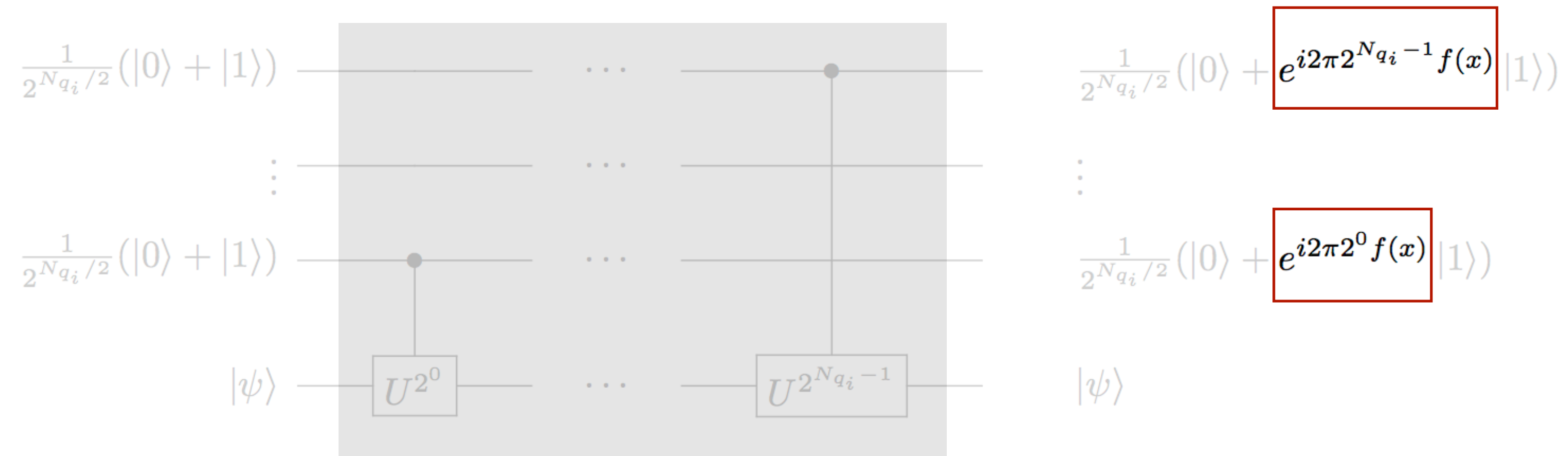
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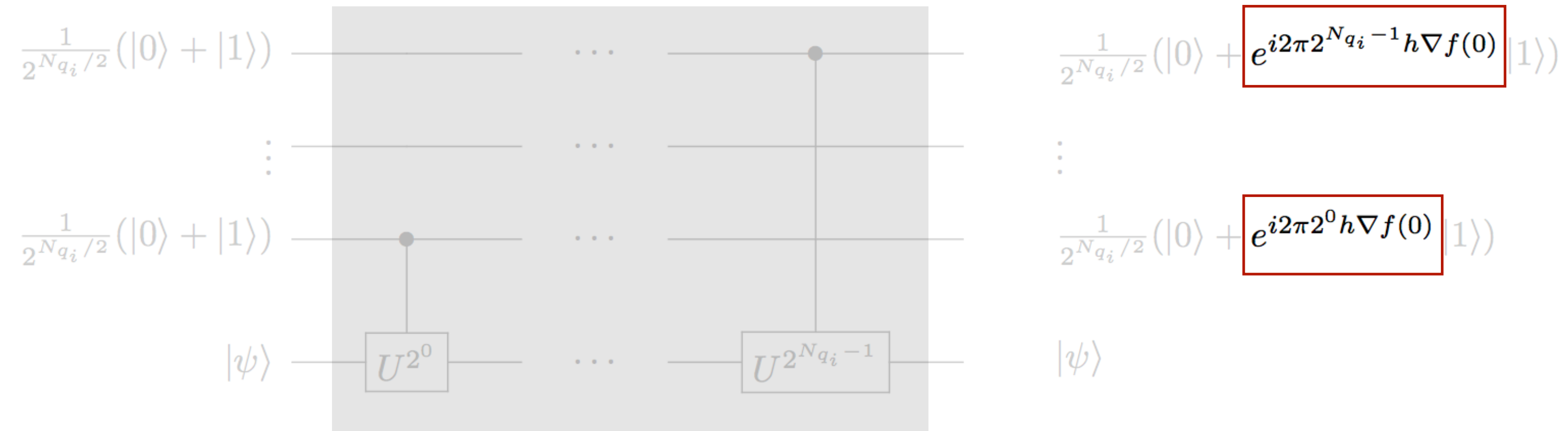
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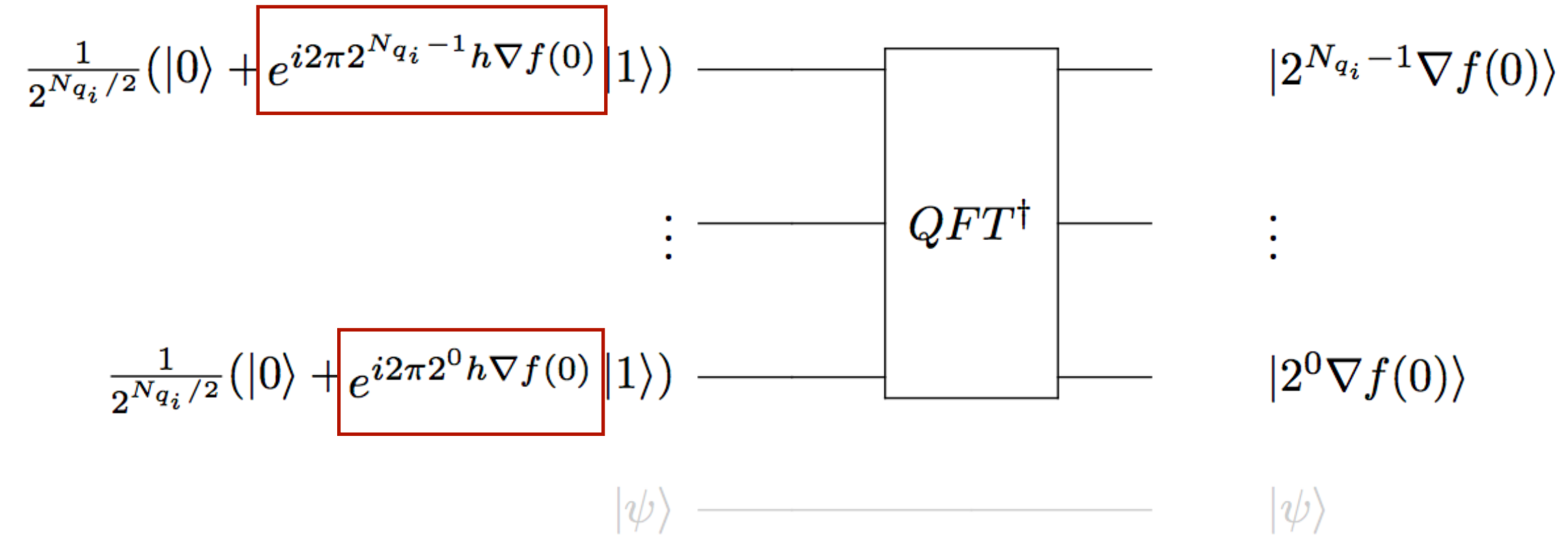
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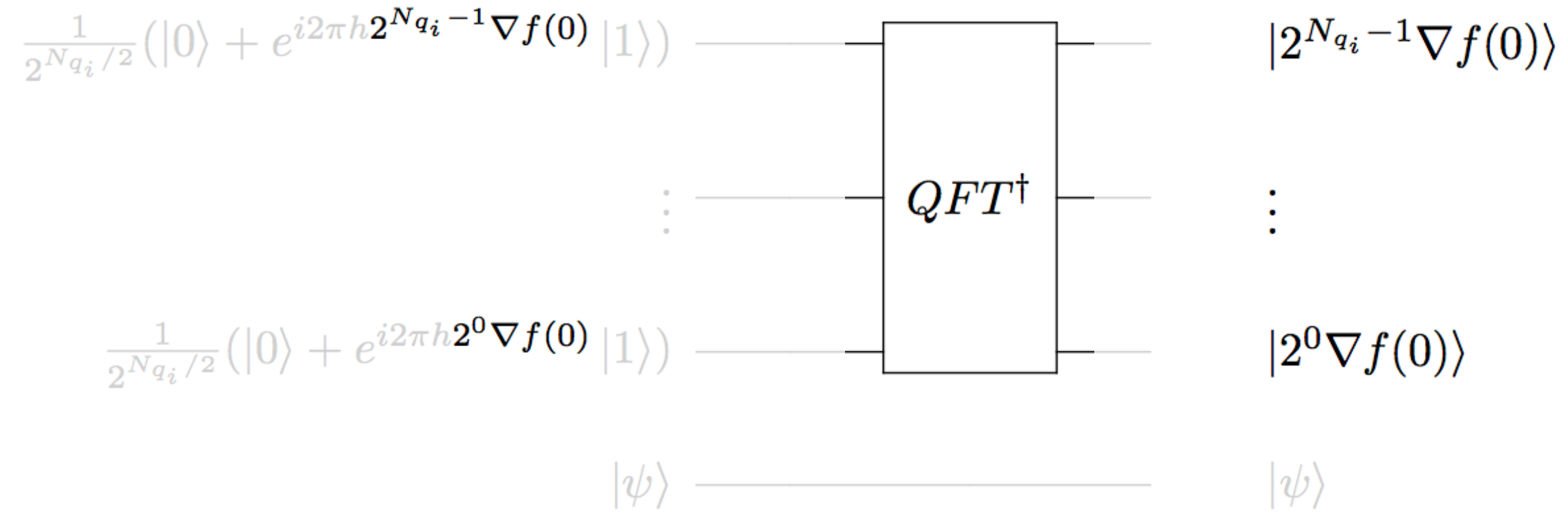
$$\nabla f(0) \approx 0.b_0 \cdots b_{n-1} \quad (6)$$

$$2^j(0.b_0 \cdots b_{n-1}) = b_0 \cdots b_j.b_{j+1} \cdots b_{n-1} \quad (7)$$

$$\begin{aligned} e^{i2\pi 2^j(0.b_0 \cdots b_{n-1})} &= e^{i2\pi b_0 \cdots b_j} e^{i2\pi b_{j+1} \cdots b_{n-1}} \\ &= e^{i2\pi b_{j+1} \cdots b_{n-1}} \end{aligned}$$

$$e^{i2\pi 2^j \nabla f(0)} \approx e^{i2\pi b_{j+1} \cdots b_{n-1}} \quad (8)$$

# phase kickback



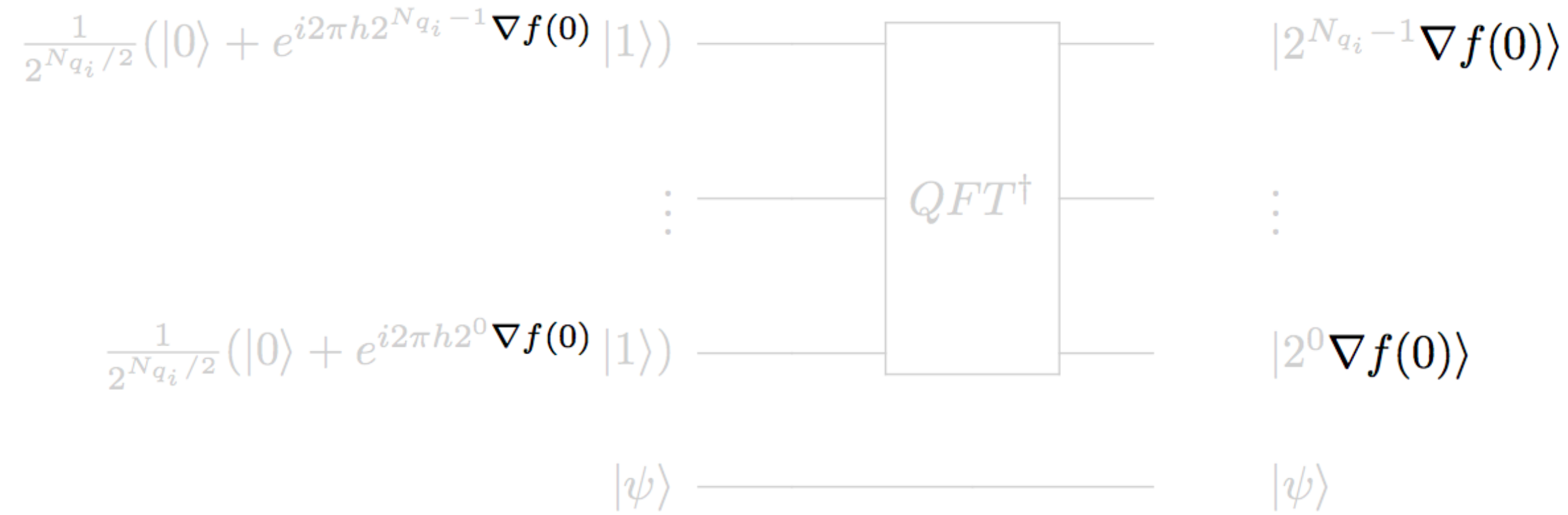
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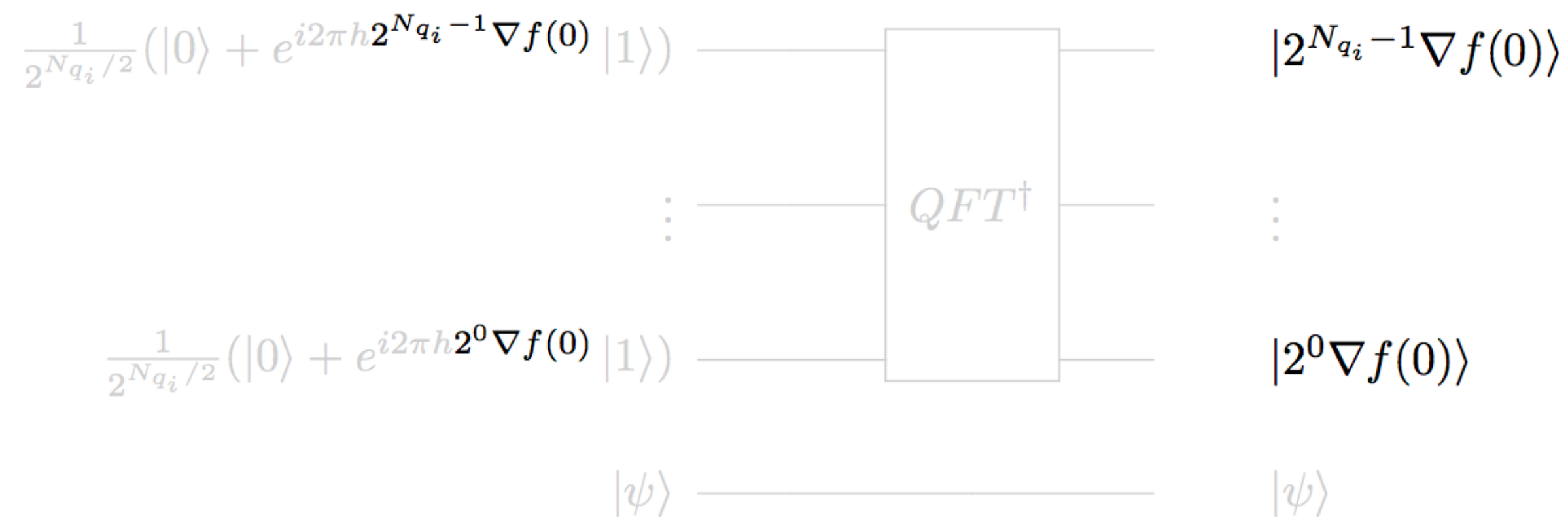
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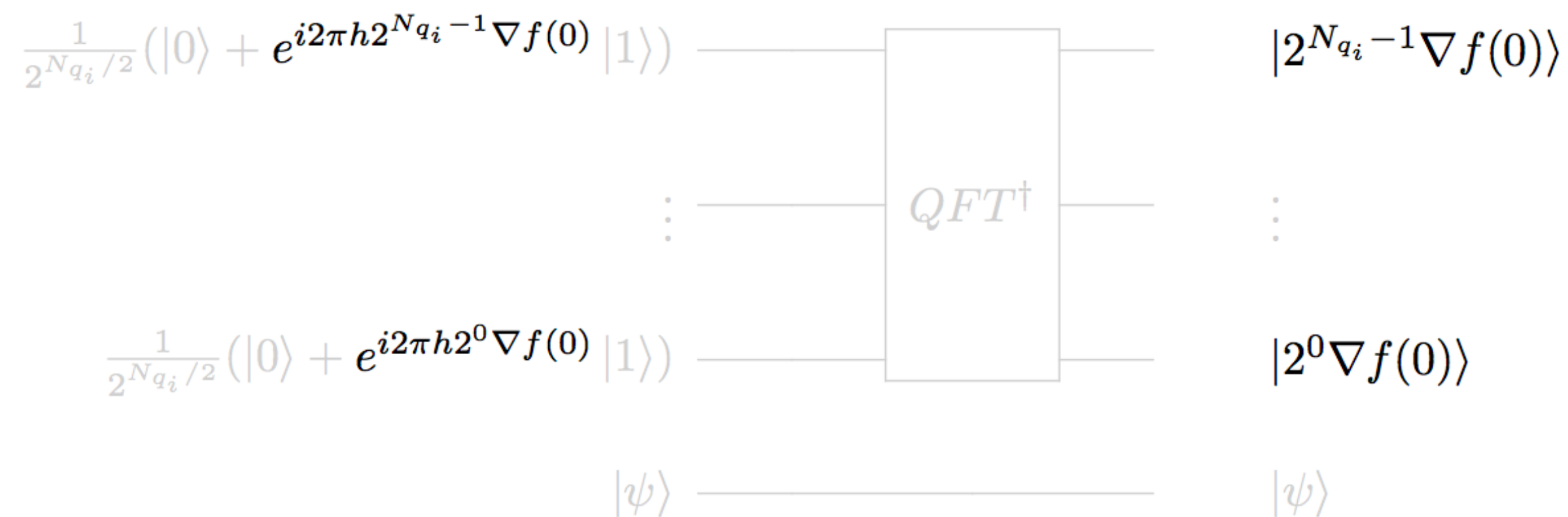
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$$\begin{aligned} e^{i2\pi 2^j(0.b_0 \cdots b_{n-1})} &= e^{i2\pi b_0 \cdots b_j} e^{i2\pi b_{j+1} \cdots b_{n-1}} \\ &= e^{i2\pi b_{j+1} \cdots b_{n-1}} \end{aligned}$$

$$e^{i2\pi 2^j \nabla f(0)} \approx e^{i2\pi b_{j+1} \cdots b_{n-1}} \quad (8)$$

# phase kickback



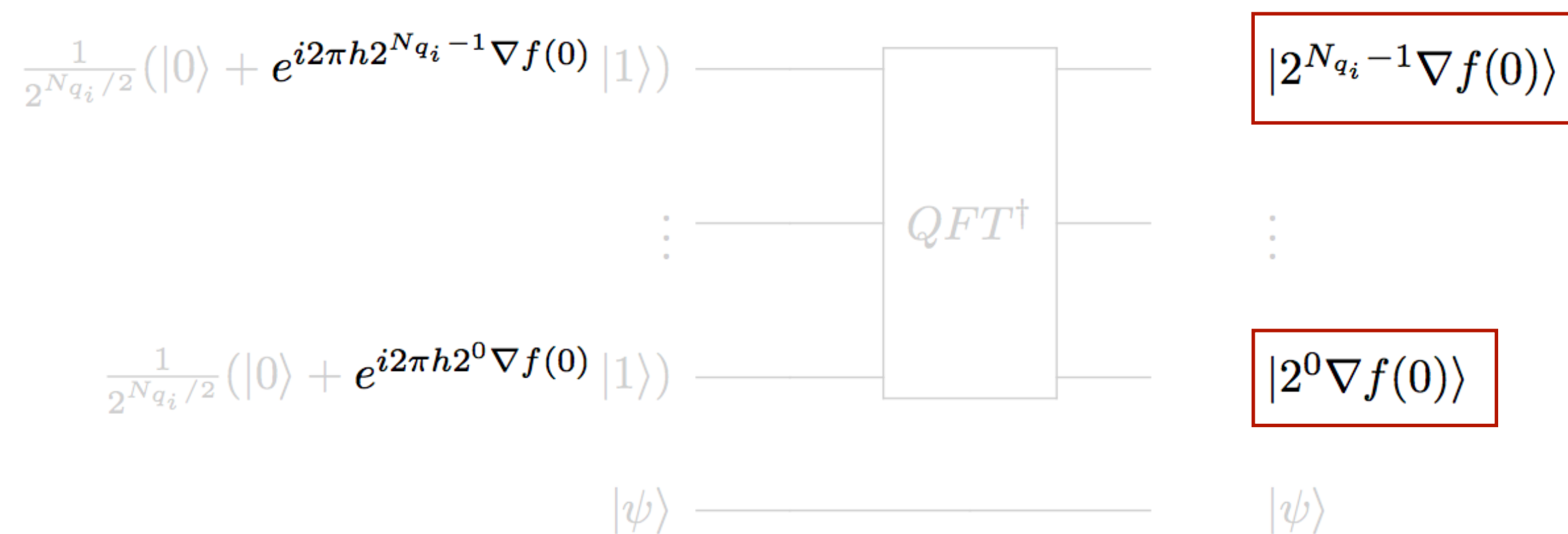
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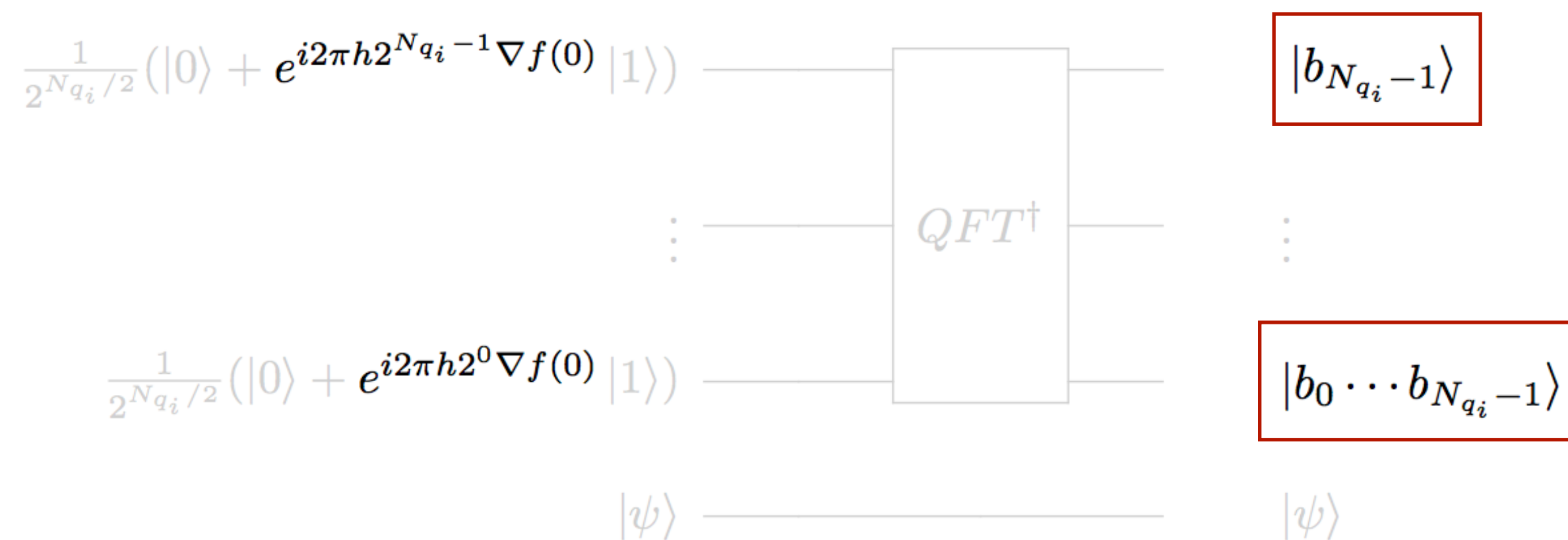
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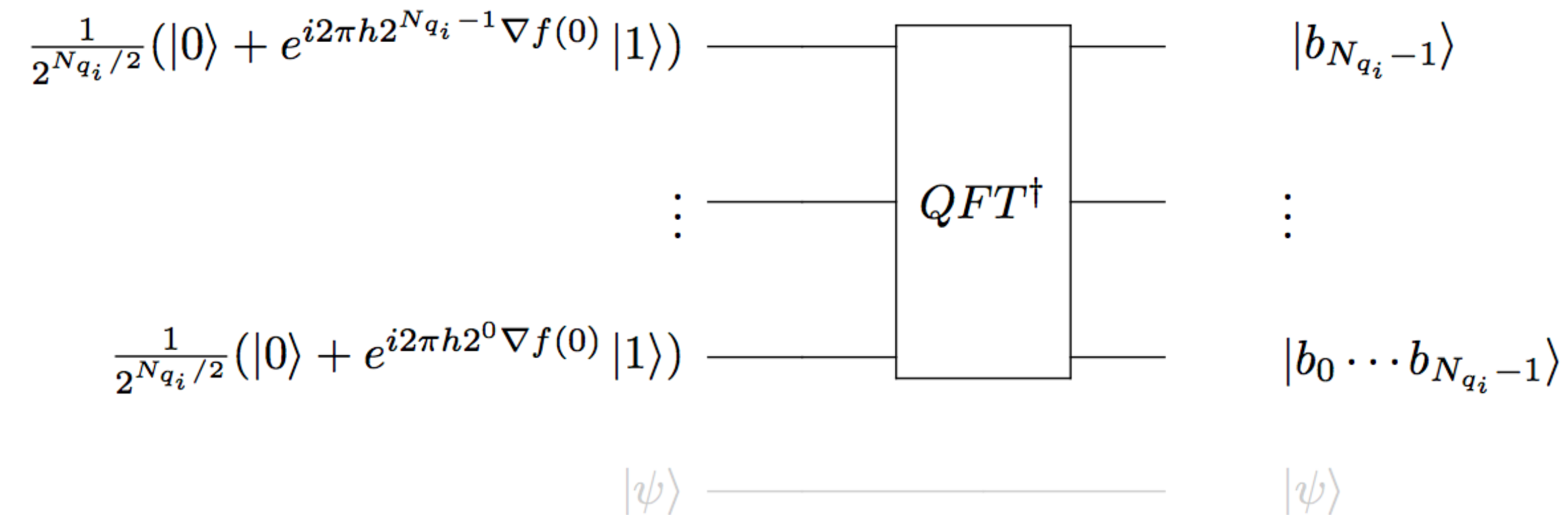
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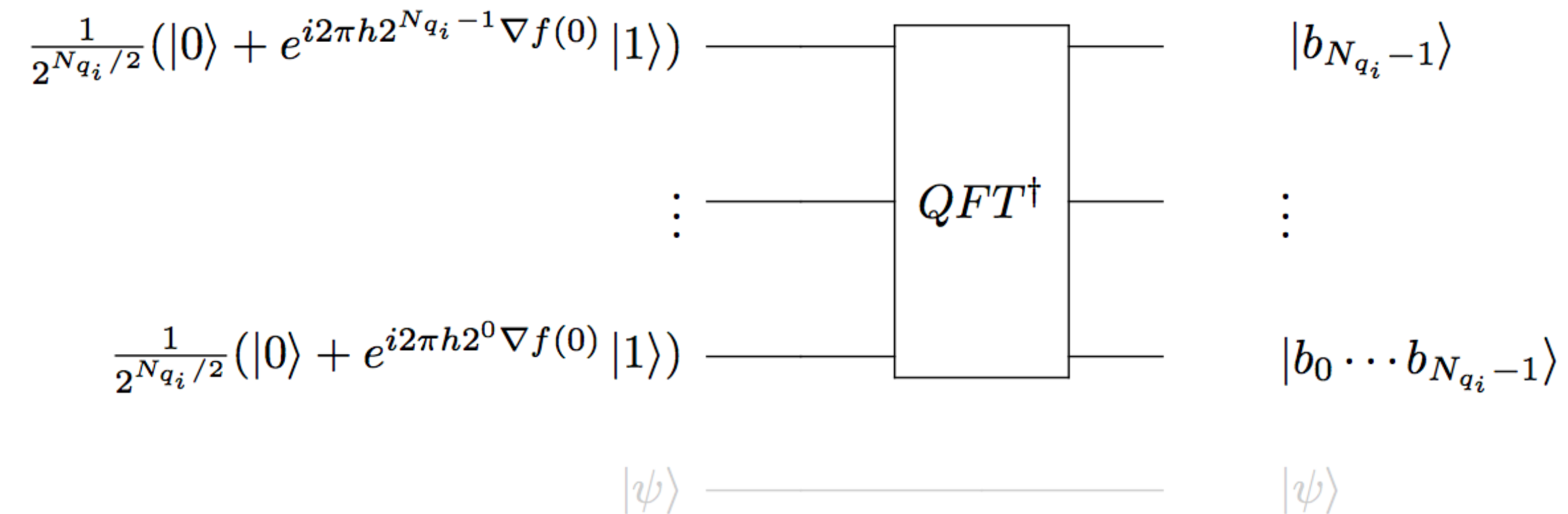
# phase kickback



```
from grove.alpha.phaseestimation.phase_estimation import controlled
from grove.qft.fourier import inverse_qft

for i in input_qubits:
    if i > 0:
        U = np.dot(U, U)
        cU = controlled(U)
        name = "c-U{0}".format(2 ** i)
        p_kickback.defgate(name, cU)
        p_kickback.inst((name, i, ancilla_qubits[0]))
# iqft to pull out fractional component of eigenphase
p_kickback += inverse_qft(input_qubits)
return p_kickback
```

# phase kickback



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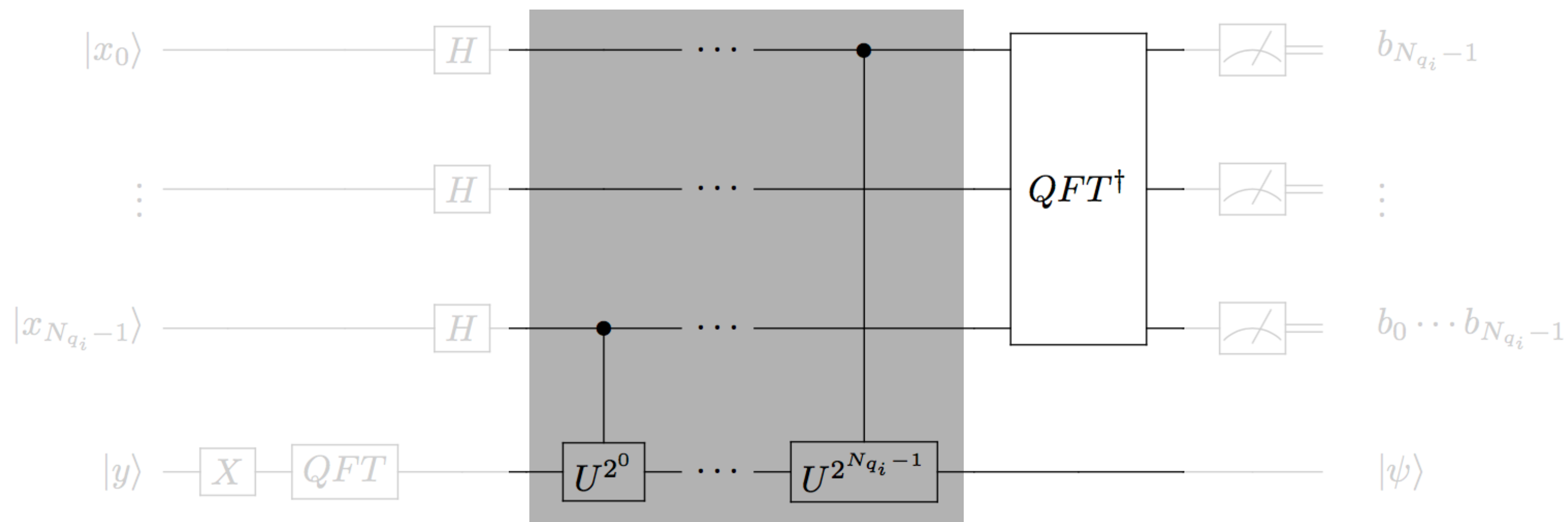
```
def phase_kickback(f_h, input_qubits, ancilla_qubits, precision):  
    """ Phase kickback of f_h
```

program	ancilla qubits	input qubits
phase kickback	U	IQFT

```
    """
```

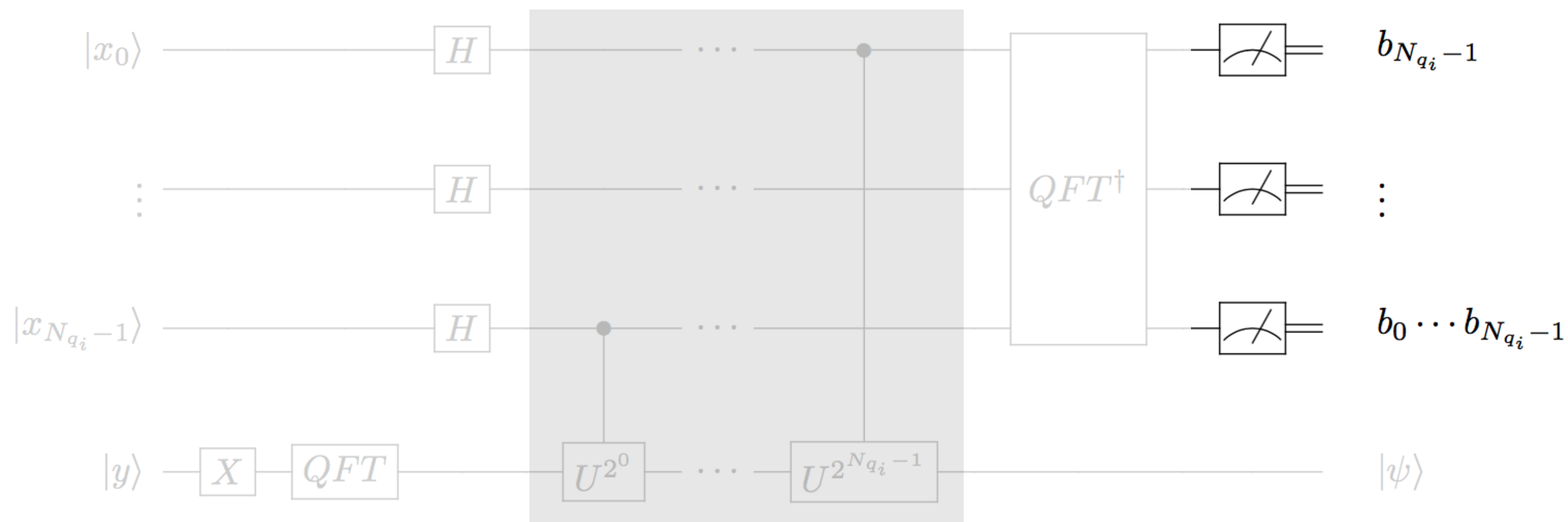
```
    # encode f_h into CPHASE gate  
    U = np.array([[1, 0],  
                  [0, np.exp(1.0j * np.pi * f_h)]])  
    p_kickback = pq.Program()  
    # apply c-U^{2^j} to ancilla register  
    for i in input_qubits:  
        if i > 0:  
            U = np.dot(U, U)  
            cU = controlled(U)  
            name = "c-U{0}".format(2 ** i)  
            p_kickback.defgate(name, cU)  
            p_kickback.inst((name, i, ancilla_qubits[0]))  
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    return p_kickback
```

# Jordan gradient estimation



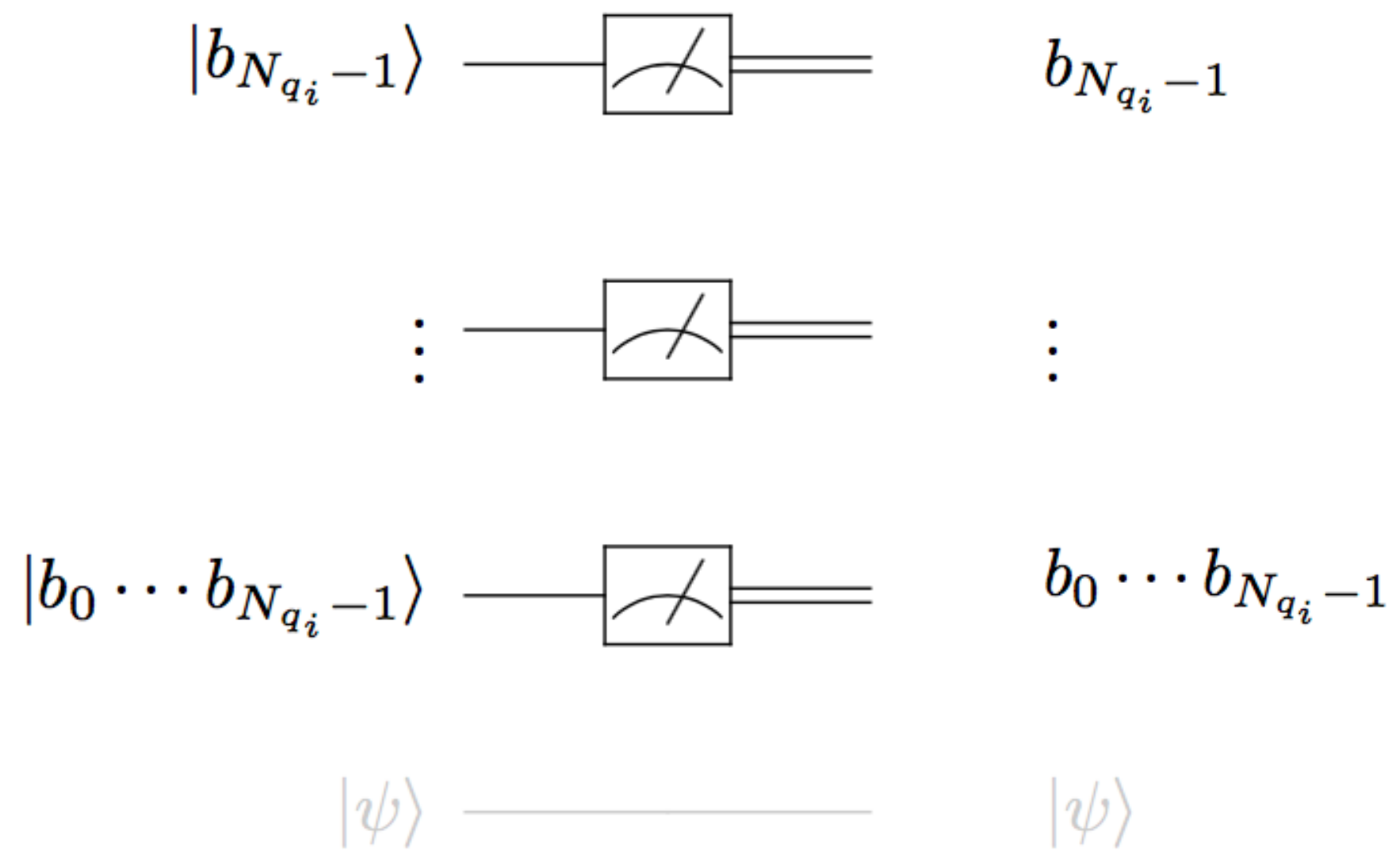
program	ancilla qubits	input qubits
initialize system	QFT, X	H
phase kickback	U	IQFT
measure	-	M

# Jordan gradient estimation



program	ancilla qubits	input qubits
initialize system	QFT, X	H
phase kickback	U	IQFT
measure	-	M

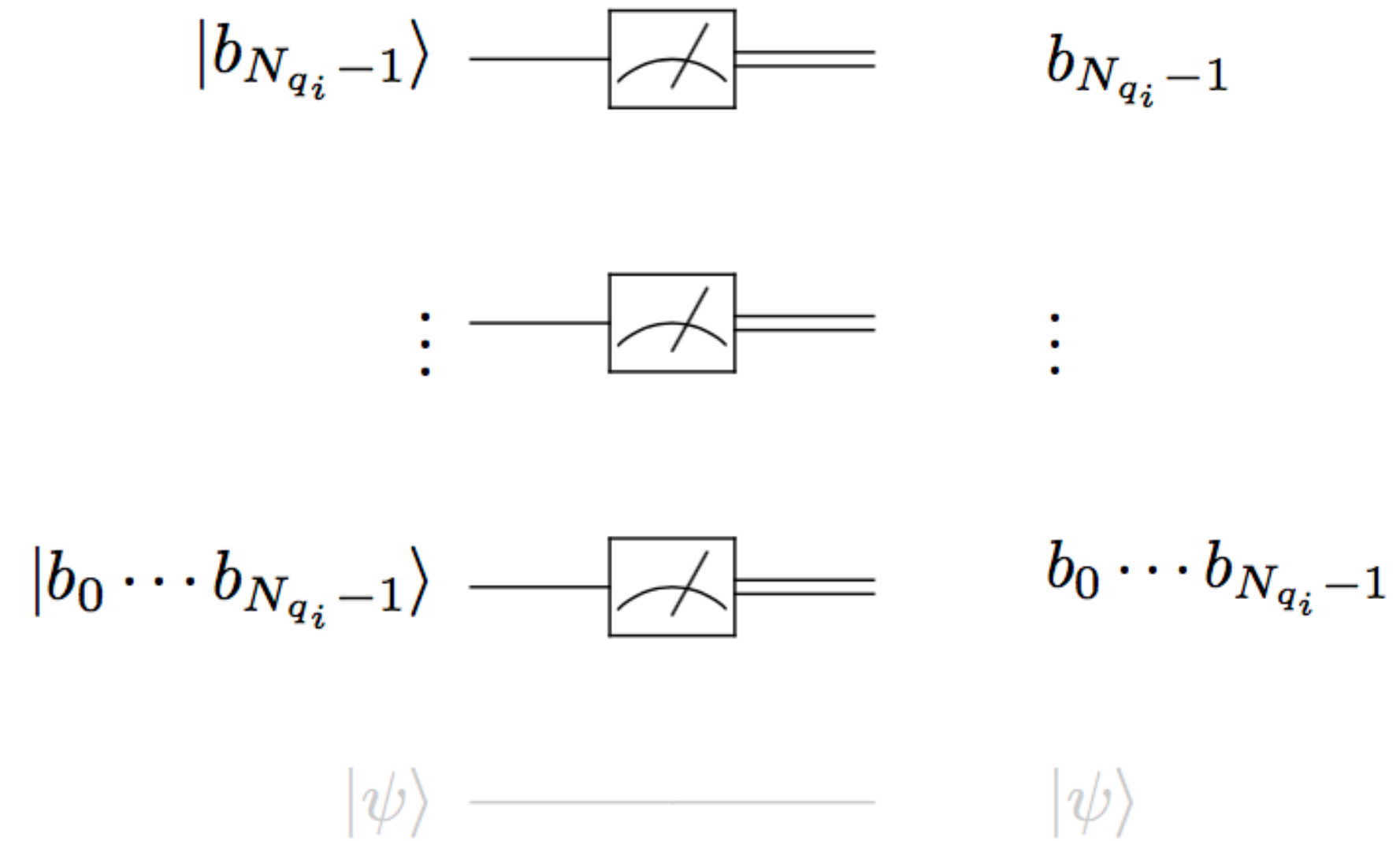
# measure



$$\nabla f(0) \approx 0.b_0 \cdots b_{n-1}$$



# measure



$$\nabla f(0) \approx 0.b_0 \cdots b_{n-1}$$

```
from pyquil.api import SyncConnection
qvm = SyncConnection()
measurement = qvm.run_and_measure(p_gradient, input_qubits)
```

# Running this algorithm

```
from jordan_gradient import gradient_estimator
p_gradient = gradient_estimator(f_h, input_qubits, ancilla_qubits,
                                precision=precision)

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measurement = qvm.run_and_measure(p_gradient, input_qubits)
```

# wrapper function

```
def gradient_estimator(f_h, input_qubits, ancilla_qubits, precision=16):  
    """ Gradient estimation via Jordan's algorithm  
    10.1103/PhysRevLett.95.050501  
  
    :param np.array f: Oracle outputs.  
    :param list input_qubit: Qubits of input registers.  
    :param list ancilla_qubits: Qubits of output register.  
    :param int precision: Bit precision of gradient.  
    :return Program p_gradient: Quil program to estimate gradient of f.  
    """  
  
    # initialize input and output registers  
    p_ic = initialize_system(input_qubits, ancilla_qubits)  
    # encode oracle values into phase  
    p_kickback = phase_kickback(f_h, input_qubits, ancilla_qubits, precision)  
    # combine steps of algorithm into one program  
    p_gradient = p_ic + p_kickback  
    return p_gradient
```

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# Demo

# Thank you

## References

### **Fast Quantum Algorithm for Numerical Gradient Estimation**

Stephen P. Jordan

10.1103/PhysRevLett.95.050501

### **Quantum Algorithm for Molecular Properties and Geometry Optimization**

Ivan Kassal, Alán Aspuru-Guzik

10.1063/1.3266959

## Code

[github.com/rigetticomputing/grove](https://github.com/rigetticomputing/grove)

[github.com/kmckiern/grove/blob/master/grove/alpha/jordan\\_gradient](https://github.com/kmckiern/grove/blob/master/grove/alpha/jordan_gradient)