$\hat{Q}\,|B\rangle$asics
Activity 3: Outer products, operators, and circuits

Resolution of the identity

In two dimensions

Suppose that $|i\rangle, |j\rangle$ form an orthonormal basis for $\mathbb{C}^2$. Show that

$$|i\rangle\langle i| + |j\rangle\langle j| = I$$

where I is the identity operator.

Note: this identity generalizes to d dimensions. If $\{|n\rangle\}_{n=0}^{d-1}$ is an orthonormal basis for $\mathbb{C}^d$, then

$$\sum_{n=0}^{d-1} |n\rangle\langle n| = I$$

Solution

A linear operator is completely defined by its action on any orthonormal basis. $\{|i\rangle, |j\rangle\}$ is orthonormal implies that

$$\langle i|i\rangle = \langle j|j\rangle = 1$$
$$\langle i|j\rangle = 0$$

Multiplication of kets is distributive, so we have

$$(|i\rangle\langle i| + |j\rangle\langle j|)\,|i\rangle = |i\rangle \underbrace{\langle i|i\rangle}_{=1} + |j\rangle \underbrace{\langle j|i\rangle}_{=0} = I\,|i\rangle$$

Similarly,

$$(|i\rangle\langle i| + |j\rangle\langle j|)\,|j\rangle = |j\rangle \underbrace{\langle i|j\rangle}_{=0} + |j\rangle \underbrace{\langle j|j\rangle}_{=1} = I\,|j\rangle$$

Since they act the same way on an orthonormal basis,

$$(|i\rangle\langle i| + |j\rangle\langle j|) = I$$

Unitary operators

Unitary operators preserve inner products

We defined a *unitary* operator as a linear operator that conserves total probability, i.e.

$$\langle\psi|\,U^\dagger U\,|\psi\rangle = \|U\,|\psi\rangle\,\|^2 = \|\,|\psi\rangle\,\|^2 = 1$$

Using the fact that this is true for an arbitrary state $|\psi\rangle$, prove that $U^\dagger U = I$, where I is the identity operator.

Hint: Consider the states $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$ and $\frac{|0\rangle+i|1\rangle}{\sqrt{2}}$.

Solution

Let $|\phi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. We can check that $\| \, |\phi\rangle \, \|^2 = 1$. By the probability-conserving property,

$$\langle\phi| U^\dagger U |\phi\rangle = 1$$

We can also expand this in terms of $|0\rangle, |1\rangle$:

$$\begin{aligned} \langle\phi| U^\dagger U |\phi\rangle &= \left(\frac{\langle 0| + \langle 1|}{\sqrt{2}}\right) U^\dagger U \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) && (1) \\ &= \frac{\langle 0| U^\dagger U |0\rangle + \langle 1| U^\dagger U |0\rangle + \langle 0| U^\dagger U |1\rangle + \langle 0| U^\dagger U |0\rangle}{2} && (2) \end{aligned}$$

By the probability-conserving property, we have $\langle 0| U^\dagger U |0\rangle = 1$ and $\langle 1| U^\dagger U |1\rangle = 1$. As a general property of the adjoint operation, we also have

$$\langle 1| U^\dagger U |0\rangle = (\langle 0| U^\dagger U |1\rangle)^*$$

Where * denotes the complex conjugate. This gives

$$\frac{\langle 0| U^\dagger U |0\rangle + \langle 1| U^\dagger U |0\rangle + \langle 0| U^\dagger U |1\rangle + \langle 1| U^\dagger U |1\rangle}{2} = \frac{2 + 2\,\mathrm{Re}(\langle 0| U^\dagger U |1\rangle)}{2} = 1 \qquad (3)$$

This top equation implies that $\mathrm{Re}(\langle 0| U^\dagger U |1\rangle) = 0$. We can repeat the same process with $|\psi\rangle = (|0\rangle + i\,|1\rangle)/\sqrt{2}$. We get

$$\begin{aligned} \langle\psi| U^\dagger U |\psi\rangle &= \left(\frac{\langle 0| - i\,\langle 1|}{\sqrt{2}}\right) U^\dagger U \left(\frac{|0\rangle + i\,|1\rangle}{\sqrt{2}}\right) && (4) \\ &= \frac{\langle 0| U^\dagger U |0\rangle - i\,\langle 1| U^\dagger U |0\rangle + i\,\langle 0| U^\dagger U |1\rangle + \langle 1| U^\dagger U |1\rangle}{2} && (5) \\ &= \frac{2 + 2i\,\mathrm{Im}(\langle 0| U^\dagger U |1\rangle)}{2} = 1 && (6) \end{aligned}$$

The last equation implies that $\mathrm{Im}(\langle 0| U^\dagger U |1\rangle) = 0$. Together, we have $\langle 0| U^\dagger U |1\rangle = 0$ and $\langle 1| U^\dagger U |0\rangle = (\langle 0| U^\dagger U |1\rangle)^* = 0$. This implies that $U^\dagger U |0\rangle = \alpha\,|0\rangle$ and $U^\dagger U |1\rangle = \beta\,|1\rangle$, where α and β are constants. Since $\langle 0| U^\dagger U |0\rangle = \alpha = 1$ and $\langle 1| U^\dagger U |1\rangle = \beta = 1$, we have $U^\dagger U |0\rangle = |0\rangle$ and $U^\dagger U |1\rangle = |1\rangle$. This shows that $U^\dagger U = I$.

Pauli-Euler identity

Consider again the Pauli-X operator, defined by $X\,|0\rangle = |1\rangle$ and $X\,|1\rangle = |0\rangle$. Recall from last time that the $X-$basis is defined as

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \qquad\qquad |-\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} \qquad (7)$$

Since $X\,|+\rangle = |+\rangle$ and $X\,|-\rangle = -\,|-\rangle$, we can consistently define $e^{i\theta X}\,|+\rangle = e^{i\theta}\,|+\rangle$ and $e^{i\theta X}\,|-\rangle = e^{-i\theta}\,|-\rangle$. Using this, show that

$$e^{i\theta X} = I\cos(\theta) + iX\sin(\theta)$$

where I is the identity operator.

Note: This holds for any operator that is self-inverse because these operators have eigenvalues ± 1, including Y, Z, and $n_x X + n_y Y + n_z Z$ where $\|(n_x, n_y, n_z)\| = 1$.

Solution

We can specify a linear operator by its action on an orthonormal basis, and $|+\rangle, |-\rangle$ forms such a basis. Using the Euler formula, we have

$$(I\cos(\theta) + iX\sin(\theta))\,|+\rangle = (\cos(\theta) + i\sin(\theta))\,|+\rangle = e^{i\theta}\,|+\rangle$$

and

$$(I\cos(\theta) + iX\sin(\theta))\,|-\rangle = (\cos(\theta) - i\sin(\theta))\,|-\rangle = e^{-i\theta}\,|-\rangle$$

This shows that $e^{i\theta X} = I\cos(\theta) + iX\sin(\theta)$.

The trace

The *trace* is a useful operation in quantum mechanics. The trace of an operator $\hat{O}$ is defined

$$\mathrm{Tr}\{\mathcal{O}\} = \langle 0|\,\mathcal{O}\,|0\rangle + \langle 1|\,\mathcal{O}\,|1\rangle$$

If we write $\mathcal{O}$ using outer products,

$$\mathcal{O} = \mathcal{O}_{00}\,|0\rangle\langle 0| + \mathcal{O}_{10}\,|1\rangle\langle 0| + \mathcal{O}_{01}\,|0\rangle\langle 1| + \mathcal{O}_{11}\,|1\rangle\langle 1|$$

we can see that $\mathrm{Tr}\{\mathcal{O}\} = \mathcal{O}_{00} + \mathcal{O}_{11}$, which is just the standard definition of the trace as the sum of diagonal elements. In d dimensions, if $\{|n\rangle\}_{n=0}^{d}$ is an orthonormal basis for $\mathbb{C}^d$, then the trace can be similarly defined as

$$\mathrm{Tr}\{\mathcal{O}\} = \sum_n \langle n|\,\mathcal{O}\,|n\rangle$$

Cyclic property of the trace

Let A and B both be operators on a $d-$dimensional complex vector space. Using the resolution of the identity, show that

$$\mathrm{Tr}\{AB\} = \mathrm{Tr}\{BA\}$$

Solution

Note that $\langle n| A |m\rangle$ is just a scalar, so it commutes with everything. Then using the defintion of the trace and resolution of the identity, we have

$$\begin{aligned}
\mathrm{Tr}\{AB\} &= \sum_{n=0}^{d-1} \langle n| AB |n\rangle && (8)\\
&= \sum_{n=0}^{d-1} \langle n| A \sum_{m=0}^{d-1} |m\rangle\langle m| B |n\rangle && (9)\\
&= \sum_{m=0}^{d-1} \sum_{n=0}^{d-1} \langle n| A |m\rangle\langle m| B |n\rangle && (10)\\
&= \sum_{m=0}^{d-1} \sum_{n=0}^{d-1} \langle m| B |n\rangle\langle n| A |n\rangle && (11)\\
&= \sum_{m=0}^{d-1} \langle m| B \sum_{n=0}^{d-1} |n\rangle\langle n| A |m\rangle && (12)\\
&= \sum_{m=0}^{d-1} \langle m| BA |m\rangle = \mathrm{Tr}\{BA\} && (13)
\end{aligned}$$

Unitary invariance of trace

If $\{|i\rangle\}_{i=0}^{d-1}$ and $\{|j\rangle\}_{j=0}^{d-1}$ are two different orthonormal bases, then the operator U such that $U|i\rangle = |j\rangle$ is unitary. Use this to show that the trace is invariant with respect to the choice of basis:

$$\mathrm{Tr}\{\mathcal{O}\} = \sum_i \langle i| \mathcal{O} |i\rangle = \sum_j \langle j| \mathcal{O} |j\rangle$$

Note: This is a slight abuse of notation because the labels i and j are both denoting indices and distinguishing between the two bases.

Solution

Let $\mathrm{Tr}\{O\} = \sum_i \langle i| \mathcal{O} |i\rangle$, and take $|j\rangle = U|i\rangle$. Since U is unitary, we have $U^\dagger U = UU^\dagger = I$. By the cyclic property of the trace,

$$\sum_j \langle j| \mathcal{O} |j\rangle = \sum_i \langle i| U^\dagger \mathcal{O} U |i\rangle = \mathrm{Tr}\left\{U^\dagger \mathcal{O} U\right\} = \mathrm{Tr}\left\{\mathcal{O} U U^\dagger\right\} = \mathrm{Tr}\{\mathcal{O}\}$$

Hello Quantum World

The Hadamard gate

The Hadamard gate is used to create superpositions, and it is defined as

$$\begin{aligned}
H|0\rangle &= |+\rangle && (14)\\
H|1\rangle &= |-\rangle && (15)
\end{aligned}$$

Make the following circuit in Qiskit: $|0\rangle - \boxed{H} - \boxed{\nearrow}$. Recall that the definition of the Z operator is $Z|0\rangle = |0\rangle$ and $Z|1\rangle = -|1\rangle$, and the expectation value is defined as $\langle Z\rangle = \langle\psi| Z |\psi\rangle$. Can you predict the expectation value $\langle Z\rangle$? Confirm your prediction by simulating in Qiskit.

Solution

For a generic state $\psi = \alpha|0\rangle + \beta|1\rangle$, the expectation value of Z is

$$\begin{aligned}\langle Z\rangle \equiv \langle\psi| Z |\psi\rangle &= (\alpha^* \langle 0| + \beta^* \langle 1|)Z(\alpha|0\rangle + \beta|1\rangle) \\ &= |\alpha|^2 \overbrace{\langle 0| Z |0\rangle}^{=1} + \alpha^*\beta \overbrace{\langle 0| Z |1\rangle}^{=0} + \alpha\beta^* \overbrace{\langle 1| Z |0\rangle}^{=0} + |\beta|^2 \overbrace{\langle 1| Z |1\rangle}^{=-1} \\ &= |\alpha|^2 - |\beta|^2\end{aligned}$$

By applying a Hadamard gate to the $|0\rangle$ state, we are left in the state $|+\rangle$, which has $\alpha = \beta = \frac{1}{\sqrt{2}}$. The expectation value of Z is then

$$|\alpha|^2 - |\beta|^2 = \frac{1}{2} - \frac{1}{2} = 0$$

We also recognize that $|\alpha|^2$ is the probability given by the Born rule of measuring $|\psi\rangle$ in the state $|0\rangle$ and $|\beta|^2$ is the probability of measuring $|\psi\rangle$ in the state $|1\rangle$. In order to compute $\langle Z\rangle$ experimentally, we can run the experiment many times and average the number of 0's and 1's to estimate $|\alpha|^2$ and $|\beta|^2$. The code in Qiskit is the following:

```
from qiskit import QuantumCircuit, execute
from qiskit.providers.aer import AerSimulator
sim = AerSimulator()
qc = QuantumCircuit(1,1)
qc.h(0)
qc.measure(0,0)
shots = 10000
counts = execute(qc, sim, shots = shots).result().get_counts()
expec_Z = (counts.get("0",0)-counts.get("1",0))/shots
```

Rotation gates

Create the following circuit in Qiskit: $|0\rangle - \boxed{R_x(\theta)} - \boxed{\nearrow}$, with the definition

$$R_x(\theta) \equiv e^{-iX\theta/2}$$

What will be the expectation value of Z as a function of θ? Make a prediction and confirm it by measuring $\langle Z\rangle$ for values of θ between 0 and 2π.

Solution

We have the Pauli-Euler identity, which gives

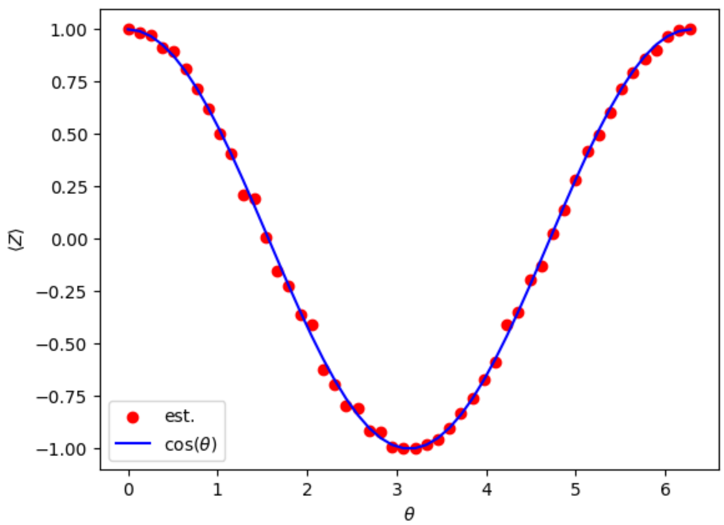
$$e^{-iX\theta/2}|0\rangle = \cos(\theta/2)|0\rangle - i\sin(\theta/2)|1\rangle$$

Using the formula $\langle Z \rangle = |\alpha|^2 - |\beta|^2$, we get

$$\langle Z \rangle = \cos^2(\theta/2) - \sin^2(\theta/2) = \cos(\theta)$$

The code we can use to test this in Qiskit is the following:

```
import numpy as np
def get_expec(theta):
    qc = QuantumCircuit(1,1)
    qc.rx(theta, 0)
    qc.measure(0,0)
    shots = 1000
    counts = execute(qc, sim, shots = shots).result().get_counts()
    return (counts.get("0",0)-counts.get("1",0))/shots
thetalist = np.linspace(0, 2*np.pi, 50)
expects = list(map(get_expec, thetalist))
```



The Bell Basis

We define the Bell basis as

$$|\Phi_1\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \qquad |\Phi_2\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$$

$$|\Phi_3\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}} \qquad |\Phi_4\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$

Come up with a circuit to prepare $|\Phi_1\rangle$. Using the definitions

$$X = |1\rangle\langle 0| + |0\rangle\langle 1| \qquad Y = i\,|1\rangle\langle 0| - i\,|0\rangle\langle 1| \qquad Z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

(a) Show that $X_1 I_2 |\Phi_1\rangle = |\Phi_3\rangle$, $Y_1 I_2 |\Phi_1\rangle = -i\,|\Phi_4\rangle$, and $Z_1 I_2 |\Phi_1\rangle = |\Phi_2\rangle$.

(b) Create a circuit that maps $|00\rangle$ to $|\Phi_1\rangle$. Now invert this circuit. What does the inverse do to $|\Phi_2\rangle, |\Phi_3\rangle$, and $|\Phi_4\rangle$?

(c) Confirm this prediction in Qiskit.

Property (a) reflects a symmetry of $|\Phi_1\rangle$ which makes it a useful resource for superdense coding and quantum teleportation, due to the fact that local (single-qubit) operators are shown to produce nonlocal (multi-qubit) changes to the state.

Part a

Using the definitions of X, Y, and Z,

$$\begin{aligned} X_1 I_2 |\Phi_1\rangle &= \frac{X_1 I_2 |00\rangle + X_1 I_2 |11\rangle}{\sqrt{2}} \\ &= \frac{|10\rangle + |01\rangle}{\sqrt{2}} = |\Phi_3\rangle \end{aligned}$$

$$\begin{aligned} Y_1 I_2 |\Phi_1\rangle &= \frac{Y_1 I_2 |00\rangle + Y_1 I_2 |11\rangle}{\sqrt{2}} \\ &= \frac{i|10\rangle - i|01\rangle}{\sqrt{2}} = -i|\Phi_4\rangle \end{aligned}$$

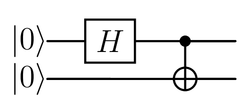
$$\begin{aligned} Z_1 I_2 |\Phi_1\rangle &= \frac{Z_1 I_2 |00\rangle + Z_1 I_2 |11\rangle}{\sqrt{2}} \\ &= \frac{|00\rangle - |11\rangle}{\sqrt{2}} = |\Phi_2\rangle \end{aligned}$$

Part b

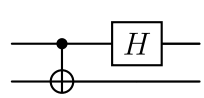
The circuit we want performs the following operation:

$$|00\rangle \mapsto \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) \mapsto \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

The first operation is a Hadamard gate on the first qubit, and the second operation is a CNOT gate controlled on the first qubit and targeting the second qubit. As a circuit,



Since $H^{-1} = H$ and $CNOT^{-1} = CNOT$, inverting the circuit is as simple as switching the order of the gates:



We can then work out the action of this inverse on the three remaining bell states:

$$CNOT\,|\Phi_2\rangle = \frac{|00\rangle - |10\rangle}{\sqrt{2}} = \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right)|0\rangle = |-\rangle|0\rangle$$

$$H_1 I_2 |-\rangle|0\rangle = |10\rangle$$

$$CNOT\,|\Phi_3\rangle = \frac{|01\rangle + |11\rangle}{\sqrt{2}} = \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right)|1\rangle = |+\rangle\,|1\rangle$$

$$H_1 I_2\,|+\rangle\,|1\rangle = |01\rangle$$

$$CNOT\,|\Phi_4\rangle = \frac{|01\rangle - |11\rangle}{\sqrt{2}} = \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right)|1\rangle = |-\rangle\,|1\rangle$$

$$H_1 I_2\,|-\rangle\,|1\rangle = |11\rangle$$

So the inverse maps $|\Phi_2\rangle \mapsto |10\rangle$, $|\Phi_3\rangle \mapsto |01\rangle$, and $|\Phi_4\rangle \mapsto |11\rangle$. In this way, a two-bit message can be encoded by applying only an operation to the first qubit. This is a quantum algorithm known as 'superdense coding.'

Part c

Note: Qiskit follows "little endian" order, so the qubits are ordered $|q_1 q_0\rangle$ instead of $|q_0 q_1\rangle$ as above.

```
qc = QuantumCircuit(2)
#prepare |Phi_1>
qc.h(0)
qc.cx(0,1)
#invert
qc.cx(0,1)
qc.h(0)
qc.measure_all()
print(execute(qc, sim).result().get_counts())
#"{'00': 1024}"
```

```
qc = QuantumCircuit(2)
#prepare |Phi_2>
qc.h(0)
qc.cx(0,1)
qc.z(0)
#invert
qc.cx(0,1)
qc.h(0)
qc.measure_all()
print(execute(qc, sim).result().get_counts())
#"{'01': 1024}"
```

```
qc = QuantumCircuit(2)
#prepare |Phi_3>
qc.h(0)
qc.cx(0,1)
qc.x(0)
#invert
qc.cx(0,1)
qc.h(0)
qc.measure_all()
print(execute(qc, sim).result().get_counts())
#"{'10': 1024}"
```

```python
qc = QuantumCircuit(2)
#prepare |Phi_4>
qc.h(0)
qc.cx(0,1)
qc.y(0)
#invert
qc.cx(0,1)
qc.h(0)
qc.measure_all()
print(execute(qc, sim).result().get_counts())
#"{'11': 1024}"
```