

PHYS 212A Exercises

Matrix Skills

■ Pauli Algebra

Pauli matrices are defined as

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1)$$

They have the following multiplication rule

$$\sigma^i \sigma^j = \delta^{ij} \mathbb{1} + i \epsilon^{ijk} \sigma^k, \quad (2)$$

for $i, j, k = 1, 2, 3$ (stands for x, y, z).

■ Vector Notation

Exc 1 | Prove $\mathbf{a} \cdot \boldsymbol{\sigma} \mathbf{b} \cdot \boldsymbol{\sigma} = \mathbf{a} \cdot \mathbf{b} \mathbb{1} + i (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}$.

Solution

Using the Einstein summation rule (repeated indices are automatically summed over)

$$\begin{aligned} \mathbf{a} \cdot \boldsymbol{\sigma} \mathbf{b} \cdot \boldsymbol{\sigma} &= a_i \sigma^i b_j \sigma^j \\ &= a_i b_j (\delta^{ij} \mathbb{1} + i \epsilon^{ijk} \sigma^k) \\ &= a_i b_i \mathbb{1} + i \epsilon^{ijk} a_i b_j \sigma^k \\ &= \mathbf{a} \cdot \mathbf{b} \mathbb{1} + i (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}. \end{aligned} \quad (3)$$

■ Commutation Relation

Exc 2 | Prove $[\mathbf{a} \cdot \boldsymbol{\sigma}, \mathbf{b} \cdot \boldsymbol{\sigma}] = 2i (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}$.

Solution

Using the result of (Exc. 1)

$$\begin{aligned} [\mathbf{a} \cdot \boldsymbol{\sigma}, \mathbf{b} \cdot \boldsymbol{\sigma}] &= \mathbf{a} \cdot \boldsymbol{\sigma} \mathbf{b} \cdot \boldsymbol{\sigma} - \mathbf{b} \cdot \boldsymbol{\sigma} \mathbf{a} \cdot \boldsymbol{\sigma} \\ &= \mathbf{a} \cdot \mathbf{b} \mathbb{1} + i (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma} - \mathbf{b} \cdot \mathbf{a} \mathbb{1} - i (\mathbf{b} \times \mathbf{a}) \cdot \boldsymbol{\sigma} \\ &= (\mathbf{a} \cdot \mathbf{b} - \mathbf{b} \cdot \mathbf{a}) \mathbb{1} + i ((\mathbf{a} \times \mathbf{b}) - (\mathbf{b} \times \mathbf{a})) \cdot \boldsymbol{\sigma} \\ &= 2i (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}. \end{aligned} \quad (4)$$

■ Trace Identity

Exc 3 | Prove $\text{Tr}(\mathbf{a} \cdot \boldsymbol{\sigma} \mathbf{b} \cdot \boldsymbol{\sigma}) = 2 \mathbf{a} \cdot \mathbf{b}$.

Solution

Using the result of (Exc. 1)

$$\begin{aligned} \text{Tr}(\mathbf{a} \cdot \boldsymbol{\sigma} \mathbf{b} \cdot \boldsymbol{\sigma}) &= \text{Tr}(\mathbf{a} \cdot \mathbf{b} \mathbf{1} + i (\mathbf{a} \times \mathbf{b}) \cdot \boldsymbol{\sigma}) \\ &= \mathbf{a} \cdot \mathbf{b} \text{Tr} \mathbf{1} + i (\mathbf{a} \times \mathbf{b}) \cdot \text{Tr} \boldsymbol{\sigma} \\ &= 2 \mathbf{a} \cdot \mathbf{b}. \end{aligned} \tag{5}$$

■ Matrix Diagonalization

Diagonalizing a matrix L corresponds to finding a unitary transformation V such that

$$L = V \Lambda V^\dagger, \tag{6}$$

where Λ is a diagonal matrix whose diagonal elements are eigenvalues and the column vectors of V are the corresponding eigenstates. For Pauli matrices, they are diagonalized by

$$\begin{aligned} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}, \\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \end{aligned} \tag{7}$$

Useful rules:

- If L is diagonalized by $L = V \Lambda V^\dagger$, $aL + b\mathbf{1}$ will be diagonalized by the same unitary V as

$$aL + b\mathbf{1} = V(a\Lambda + b\mathbf{1})V^\dagger. \tag{8}$$

Rescaling the matrix by a constant and shifting the diagonal by identity matrix do not change the eigenvectors.

- If L can be separated into blocks L_1 and L_2 with $L_1 = V_1 \Lambda_1 V_1^\dagger$ and $L_2 = V_2 \Lambda_2 V_2^\dagger$, then it can be diagonalized in each block separately

$$\begin{aligned} L = \begin{pmatrix} L_1 & 0 \\ 0 & L_2 \end{pmatrix} &= \begin{pmatrix} V_1 \Lambda_1 V_1^\dagger & 0 \\ 0 & V_2 \Lambda_2 V_2^\dagger \end{pmatrix} \\ &= \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix} \begin{pmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{pmatrix} \begin{pmatrix} V_1^\dagger & 0 \\ 0 & V_2^\dagger \end{pmatrix}. \end{aligned} \tag{9}$$

- If L can be decomposed to **tensor product** of L_1 and L_2 with $L_1 = V_1 \Lambda_1 V_1^\dagger$ and $L_2 = V_2 \Lambda_2 V_2^\dagger$, then it can be diagonalized in each tensor factor separately

$$\begin{aligned}
L &= L_1 \otimes L_2 \\
&= (V_1 \Lambda_1 V_1^\dagger) \otimes (V_2 \Lambda_2 V_2^\dagger) \\
&= (V_1 \otimes V_2) (\Lambda_1 \otimes \Lambda_2) (V_1 \otimes V_2)^\dagger.
\end{aligned} \tag{10}$$

■ Adding Identity

**Exc
4**

Diagonalize the matrix
 $\begin{pmatrix} 3 & 2 \\ 2 & 3 \end{pmatrix}$.

Solution

The matrix can be viewed as

$$\begin{pmatrix} 3 & 2 \\ 2 & 3 \end{pmatrix} = 3 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + 2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = 3 \mathbf{1} + 2 \sigma^x. \tag{11}$$

Use Eq. (8). Eigenvalues: 3 ± 2 . Eigenvectors:

$$|3 \pm 2\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}. \tag{12}$$

■ Block Diagonalization (I)

**Exc
5**

Diagonalize the matrix
 $\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 2 & 0 \end{pmatrix}$.

The matrix contains two blocks.

Solution

The matrix is of the form

$$\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \text{ with } A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, B = \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}. \tag{13}$$

For A , eigenvalues: ± 1 , eigenvectors: $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$. For B , eigenvalues: ± 2 , eigenvectors: $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$.

Put together, for the original matrix, eigenvalues: $\pm 1, \pm 2$. Eigenvectors:

$$|\pm 1\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \\ 0 \\ 0 \end{pmatrix}, |\pm 2\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ \pm 1 \end{pmatrix}. \tag{14}$$

■ Block Diagonalization (II)

**Exc
6**

Diagonalize the matrix

$$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 0 & 4 & 0 & 3 \\ 2 & 0 & 1 & 0 \\ 0 & 3 & 0 & 4 \end{pmatrix}$$

The matrix also contains two “blocks” that can be diagonalized separately, can you identify the blocks?

Solution

The two “blocks” are interlacing with each other

$$\begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \text{ and } \begin{pmatrix} 4 & 3 \\ 3 & 4 \end{pmatrix}. \quad (15)$$

By swapping the 2nd and 3rd basis, the matrix can be rearranged to the block diagonal form explicitly, but one need to remember to convert to the original basis back after obtaining the eigenvectors.

Eigenvalues: 1 ± 2 , 4 ± 3 . Eigenvectors:

$$|1 \pm 2\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ \pm 1 \\ 0 \end{pmatrix}, \quad |4 \pm 3\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \pm 1 \end{pmatrix}. \quad (16)$$

■ Dark State

**Exc
7**

Diagonalize the matrix

$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

The matrix corresponds to an operator

$$|1\rangle\langle 2| + |1\rangle\langle 3| + |2\rangle\langle 1| + |3\rangle\langle 1|, \quad (17)$$

which can be factorized as

$$\sqrt{2} |1\rangle \frac{\langle 2| + \langle 3|}{\sqrt{2}} + \sqrt{2} \frac{|2\rangle + |3\rangle}{\sqrt{2}} \langle 1|, \quad (18)$$

meaning that the state $|1\rangle$ only hybridize with the state $\frac{|2\rangle + |3\rangle}{\sqrt{2}}$, and the remaining orthogonal state $\frac{|2\rangle - |3\rangle}{\sqrt{2}}$ is “dark”.

Solution

Take the new basis

$$|1\rangle, \frac{|2\rangle + |3\rangle}{\sqrt{2}}, \frac{|2\rangle - |3\rangle}{\sqrt{2}}, \quad (19)$$

The matrix can be represented as

$$\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (20)$$

Meaning that the original matrix can factorized to

$$\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}. \quad (21)$$

Now Eq. (20) can be further diagonalized as

$$\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & -\sqrt{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (22)$$

substitute into Eq. (21), we have

$$\begin{aligned} \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & -\sqrt{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{2} & \frac{-1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & -\sqrt{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}. \end{aligned} \quad (23)$$

Eq. (23) implies the eigenvalues: $\pm \sqrt{2}$, 0 and the eigenvectors:

$$|\sqrt{2}\rangle \simeq \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \quad |-\sqrt{2}\rangle \simeq \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{2} \\ -\frac{1}{2} \end{pmatrix}, \quad |0\rangle \simeq \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}. \quad (24)$$

■ Tensor Product Operator

Exc
8

Diagonalize the matrix

$$\begin{pmatrix} 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 \\ 1 & 2 & 0 & 0 \end{pmatrix}$$

Solution

The matrix can be written as

$$A \otimes B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \quad (25)$$

For A , eigenvalues ± 1 with eigenvectors $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$. For B , eigenvalues 2 ± 1 with eigenvectors $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$.

Put together, the eigenvalues should be $(\pm 1) \times (2 \pm 1) = +3, +1, -1, -3$

$$\begin{aligned} | +3 \rangle &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \\ | +1 \rangle &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \\ | -1 \rangle &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}, \\ | -3 \rangle &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}. \end{aligned} \quad (26)$$

■ Matrix Exponential

Matrix exponential is important for calculating unitary evolution $U(t) = e^{-i H t}$.

- Block diagonalized matrix can be exponentiated in each block

$$\exp \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} = \begin{pmatrix} \exp A & 0 \\ 0 & \exp B \end{pmatrix}. \quad (27)$$

■ Exponential of Diagonal Matrices

If H is diagonal

$$H = \begin{pmatrix} E_1 & & \\ & E_2 & \\ & & \ddots \end{pmatrix}, \quad (28)$$

the matrix exponential simply exponentiates each diagonal element

$$e^{-i H t} = \begin{pmatrix} e^{-i E_1 t} & & \\ & e^{-i E_2 t} & \\ & & \ddots \end{pmatrix}. \quad (29)$$

**Exc
9**

Construct the unitary evolution operator generated by the following Hamiltonian

$$H = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Solution

Note that H is diagonal,

$$e^{-i H t} = \begin{pmatrix} e^{-i 0 t} & 0 & 0 \\ 0 & e^{-i 1 t} & 0 \\ 0 & 0 & e^{-i (-1) t} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{-i t} & 0 \\ 0 & 0 & e^{+i t} \end{pmatrix}. \quad (30)$$

■ Matrix Exponential by Diagonalization

**Exc
10**

Construct the unitary evolution operator generated by the following Hamiltonian

$$H = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

Solution

First find the eigen values and eigen vectors of H . Note that $H = \mathbf{1} + \sigma^x$. Following the approach in (Exc. 4), the eigen values are 1 ± 1 , and the corresponding eigen vectors are

$$|1 \pm 1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}. \quad (31)$$

This means that H can be diagonalized by the unitary matrix

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (32)$$

such that

$$H = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = V \Lambda V^\dagger. \quad (33)$$

The unitary evolution operator is given by

$$e^{-i H t} = e^{-i V \Lambda V^\dagger t} = V e^{-i \Lambda t} V^\dagger. \quad (34)$$

Because Λ is diagonal, its matrix exponential is simply

$$e^{-i \Lambda t} = \begin{pmatrix} e^{-2 i t} & 0 \\ 0 & 1 \end{pmatrix}, \quad (35)$$

therefore

$$\begin{aligned} e^{-i H t} &= V e^{-i \Lambda t} V^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} e^{-2 i t} & 0 \\ 0 & 1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} e^{-2 i t} + 1 & e^{-2 i t} - 1 \\ e^{-2 i t} - 1 & e^{-2 i t} + 1 \end{pmatrix}. \end{aligned} \quad (36)$$

Use *Mathematica* to verify the result

```
MatrixExp[-i t {{1, 1}, {1, 1}}]
{ {1/2 + 1/2 e^{-2 i t}, -1/2 + 1/2 e^{-2 i t}}, { -1/2 + 1/2 e^{-2 i t}, 1/2 + 1/2 e^{-2 i t}} }
```

■ Matrix Exponential by Taylor Expansion

For matrices that squares to identity, i.e. $H^2 = \mathbf{1}$, its matrix exponential can be calculated by Taylor expansion

$$\begin{aligned} e^{-i H t} &= \sum_{k=0}^{\infty} \frac{(-i H t)^k}{k!} \\ &= \sum_{k=0}^{\infty} \frac{(-i H t)^{2k}}{(2k)!} + \sum_{k=0}^{\infty} \frac{(-i H t)^{2k+1}}{(2k+1)!} \\ &= \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k}}{(2k)!} H^{2k} - i \sum_{k=0}^{\infty} \frac{(-1)^k t^{2k+1}}{(2k+1)!} H^{2k+1} \\ &= \cos t \mathbf{1} - i \sin t H. \end{aligned} \quad (37)$$

**Exc
11**

Construct the unitary evolution operator generated by the following Hamiltonian

$$H = \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}.$$

Solution

Note that

$$H^2 = \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix} = \begin{pmatrix} 9 & 0 & 0 \\ 0 & 9 & 0 \\ 0 & 0 & 9 \end{pmatrix} = 9 \mathbf{1}, \quad (38)$$

which is proportional to $\mathbf{1}$. We can define $\tilde{H} = H/3$, such that

$$\tilde{H}^2 = \left(\frac{H}{3}\right)^2 = \frac{1}{9} H^2 = \mathbf{1}. \quad (39)$$

Then we can use Eq. (37) to compute the matrix exponential

$$\begin{aligned} e^{-i H t} &= e^{-i (H/3) 3 t} = e^{-i \tilde{H} 3 t} \\ &= \cos(3 t) \mathbf{1} - i \sin(3 t) \tilde{H} \\ &= \cos(3 t) \mathbf{1} - \frac{i}{3} \sin(3 t) H \\ &= \cos(3 t) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{i}{3} \sin(3 t) \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix} \\ &= \begin{pmatrix} \cos(3 t) + \frac{i}{3} \sin(3 t) & -\frac{2i}{3} \sin(3 t) & -\frac{2i}{3} \sin(3 t) \\ -\frac{2i}{3} \sin(3 t) & \cos(3 t) + \frac{i}{3} \sin(3 t) & -\frac{2i}{3} \sin(3 t) \\ -\frac{2i}{3} \sin(3 t) & -\frac{2i}{3} \sin(3 t) & \cos(3 t) + \frac{i}{3} \sin(3 t) \end{pmatrix} \end{aligned} \quad (40)$$

Use *Mathematica* to verify the result

```
Simplify@ExpToTrig@MatrixExp[-i t {{-1, 2, 2}, {2, -1, 2}, {2, 2, -1}}]
```

$$\begin{aligned} &\left\{ \left\{ \cos[3 t] + \frac{1}{3} i \sin[3 t], -\frac{2}{3} i \sin[3 t], -\frac{2}{3} i \sin[3 t] \right\}, \right. \\ &\left\{ -\frac{2}{3} i \sin[3 t], \cos[3 t] + \frac{1}{3} i \sin[3 t], -\frac{2}{3} i \sin[3 t] \right\}, \\ &\left. \left\{ -\frac{2}{3} i \sin[3 t], -\frac{2}{3} i \sin[3 t], \cos[3 t] + \frac{1}{3} i \sin[3 t] \right\} \right\} \end{aligned}$$

■ Exponential of Pauli Matrices

The following formula will be useful

$$\exp(i t \mathbf{n} \cdot \boldsymbol{\sigma}) = \cos t \mathbf{1} + i \sin t \mathbf{n} \cdot \boldsymbol{\sigma}, \quad (41)$$

given that \mathbf{n} is a **unit vector**.

Exc 12 Show that if there is no factor i on the exponent, we should have $\exp(\tau \mathbf{n} \cdot \boldsymbol{\sigma}) = \cosh \tau \mathbb{1} + \sinh \tau \mathbf{n} \cdot \boldsymbol{\sigma}$.

This is known as the “imaginary time” evolution, which is *not* unitary.

Solution

Starting from Eq. (41) and replacing real time by imaginary time $t \rightarrow -i\tau$. Then using $\cos(ix) = \cosh x$, $\sin(ix) = i \sinh x$, the remaining proof is straight forward.

■ Block Exponential

Exc 13 Construct the unitary evolution operator generated by the following Hamiltonian

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Solution

The middle 2×2 block takes the form of σ^y , its exponentiation is given by

$$e^{-it\sigma^y} = \cos t \mathbb{1} - i \sin t \sigma^y = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix} \quad (42)$$

Embed into the 4×4 matrix, e^{-itH} reads

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos t & -\sin t & 0 \\ 0 & \sin t & \cos t & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (43)$$

Use *Mathematica* to verify the result

```
MatrixExp[-i t {{0, 0, 0, 0}, {0, 0, -i, 0}, {0, i, 0, 0}, {0, 0, 0, 0}}]
{{1, 0, 0, 0}, {0, Cos[t], -Sin[t], 0}, {0, Sin[t], Cos[t], 0}, {0, 0, 0, 1}}
```

■ Matrix Log

Matrix logarithm is useful in calculating entropy (like $-\text{Tr} \rho \ln \rho$). The way to calculate matrix log is to first bring the matrix to its diagonal form $L = V \Lambda V^\dagger$, apply the log to the diagonal matrix $\Lambda \rightarrow \ln \Lambda$, and then transform back to the original basis, such that

$$\ln L = \ln(V \Lambda V^\dagger) = V (\ln \Lambda) V^\dagger. \quad (44)$$

As Λ is a diagonal matrix, its log is just the log of the diagonal elements

$$\ln \Lambda = \ln \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \ddots \end{pmatrix} = \begin{pmatrix} \ln \lambda_1 & & \\ & \ln \lambda_2 & \\ & & \ddots \end{pmatrix}. \quad (45)$$

■ 2x2 Matrix Log

Exc
14

Calculate the following matrix log

$$\ln \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

Solution

First bring the matrix to its diagonal form by unitary transformation

$$\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 2+1 & 0 \\ 0 & 2-1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (46)$$

According to Eq. (44) and Eq. (45)

$$\begin{aligned} \ln \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \ln(2+1) & 0 \\ 0 & \ln(2-1) \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \ln 3 & 0 \\ 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{\ln 3}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \end{aligned} \quad (47)$$

In fact, the matrix log can be calculated in *Mathematica* by `MatrixLog`

```
MatrixLog[{{2, 1}, {1, 2}}]
```

$$\left\{ \left\{ \frac{\text{Log}[3]}{2}, \frac{\text{Log}[3]}{2} \right\}, \left\{ \frac{\text{Log}[3]}{2}, \frac{\text{Log}[3]}{2} \right\} \right\}$$

■ Log of Single-Qubit Density Matrix

Exc
15

A single-qubit density matrix generally takes the form of

$$\rho = \frac{1}{2} (1 + \mathbf{m} \cdot \boldsymbol{\sigma}),$$

where \mathbf{m} is a three-component real vector. Calculate $\ln \rho$.

Solution

Rewrite the \mathbf{m} vector as its magnitude multiplying its direction

$$\mathbf{m} = |\mathbf{m}| \hat{\mathbf{m}}, \quad (48)$$

where

$$|\mathbf{m}| = \sqrt{m_1^2 + m_2^2 + m_3^2}, \quad \hat{\mathbf{m}} = \frac{(m_1, m_2, m_3)}{\sqrt{m_1^2 + m_2^2 + m_3^2}}. \quad (49)$$

The density matrix has two eigenvalues, with the corresponding projection operators

$$p_{\pm} = \frac{1 \pm |\mathbf{m}|}{2}, \quad P_{\pm} = \frac{1}{2} (\mathbb{1} \pm \hat{\mathbf{m}} \cdot \boldsymbol{\sigma}), \quad (50)$$

such that

$$\rho = p_+ P_+ + p_- P_- . \quad (51)$$

Then the log simply applies to the eigenvalues,

$$\begin{aligned} \ln \rho &= (\ln p_+) P_+ + (\ln p_-) P_- \\ &= \frac{1}{2} (\mathbb{1} + \hat{\mathbf{m}} \cdot \boldsymbol{\sigma}) \ln \frac{1 + |\mathbf{m}|}{2} + \frac{1}{2} (\mathbb{1} - \hat{\mathbf{m}} \cdot \boldsymbol{\sigma}) \ln \frac{1 - |\mathbf{m}|}{2} \\ &= \left(\ln \frac{\sqrt{1 - |\mathbf{m}|^2}}{2} \right) \mathbb{1} + \left(\ln \sqrt{\frac{1 + |\mathbf{m}|}{1 - |\mathbf{m}|}} \right) \hat{\mathbf{m}} \cdot \boldsymbol{\sigma}. \end{aligned} \quad (52)$$

■ Projection Operator

Projection operator is essential in understanding measurement. The projection operator associated with observing $L = \lambda$ is given by

$$P(L = \lambda) = \sum_i |\lambda_i\rangle \delta(\lambda_i - \lambda) \langle \lambda_i|. \quad (53)$$

■ Construct by Diagonalization

**Exc
16**

Given an observable L described by

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

construct the projection operator corresponds to $L = 1$ and $L = -1$.

Solution

First diagonalize L , find eigenvalues and corresponding eigenvectors.

Eigenvalue 1 has two corresponding eigenvectors

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \quad (54)$$

they can be arranged in a rectangular matrix

$$V_1 = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix}. \quad (55)$$

The projection operator for $L = 1$ is given by

$$P(L = 1) = V_1 V_1^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix}. \quad (56)$$

Eigenvalue -1 has only one eigenvector

$$V_{-1} = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}. \quad (57)$$

The projection operator for $L = -1$ is given by

$$P(L = -1) = V_{-1} V_{-1}^\dagger = \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1/2 & -1/2 \\ 0 & -1/2 & 1/2 \end{pmatrix}. \quad (58)$$

■ Algebraic Construction

If operator L has eigenvalues $\lambda_1, \lambda_2, \lambda_3, \dots$, the projection operator for $L = \lambda_i$ will be proportional to

$$P(L = \lambda_i) \propto \prod_{j \neq i} (L - \lambda_j \mathbf{1}), \quad (59)$$

as the product vanishes when L takes any eigenvalue other than λ_i .

**Exc
17**

Given an observable L described by

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

construct the projection operator corresponds to $L = 1$.

Solution

Notice that L has eigenvalues 1 (3-fold) and -3 (1-fold), the projection operator for $L = 1$ is given by

$$P(L = 1) \propto L - (-3) \mathbf{1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 2 & 0 \\ 0 & 2 & 2 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix} \quad (60)$$

To properly normalize $P(L = 1)$, we require that $\text{Tr } P(L = 1) = 3$ because the eigenvalue 1 has 3-fold degeneracy, so

$$P(L=1) = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}. \quad (61)$$

■ Pauli Observable

For Pauli observable $\mathbf{n} \cdot \boldsymbol{\sigma}$ (where \mathbf{n} is a unit vector), the projection operator is given by

$$P(\mathbf{n} \cdot \boldsymbol{\sigma} = \pm 1) = \frac{\mathbb{1} \pm \mathbf{n} \cdot \boldsymbol{\sigma}}{2}. \quad (62)$$

**Exc
18**

Prove the result in Eq. (62).

Solution

Using the algebraic construction method in Eq. (59).

Note that regardless of the direction of the unit vector \mathbf{n} , $\mathbf{n} \cdot \boldsymbol{\sigma}$ always has two eigen values: ± 1 . Therefore

$$P(\mathbf{n} \cdot \boldsymbol{\sigma} = \pm 1) \propto \mathbf{n} \cdot \boldsymbol{\sigma} - (\mp 1) \mathbb{1} = \mathbf{n} \cdot \boldsymbol{\sigma} \pm \mathbb{1}. \quad (63)$$

To properly normalize $P(\mathbf{n} \cdot \boldsymbol{\sigma} = \pm 1)$, we require $\text{Tr } P(\mathbf{n} \cdot \boldsymbol{\sigma} = \pm 1) = 1$, since both eigen space is 1 dimensional, thus

$$P(\mathbf{n} \cdot \boldsymbol{\sigma} = \pm 1) = \frac{\mathbf{n} \cdot \boldsymbol{\sigma} \pm \mathbb{1}}{\text{Tr}(\mathbf{n} \cdot \boldsymbol{\sigma} \pm \mathbb{1})} = \frac{\mathbf{n} \cdot \boldsymbol{\sigma} \pm \mathbb{1}}{\pm 2} = \frac{\mathbb{1} \pm \mathbf{n} \cdot \boldsymbol{\sigma}}{2}. \quad (64)$$

■ Singlet v.s. Triplet Projection

**Exc
19**

Consider a two-qubit system with the following Hamiltonian

$$H = \boldsymbol{\sigma}_A \cdot \boldsymbol{\sigma}_B.$$

If the system is initially in the $|\uparrow\downarrow\rangle$ state, what are the possible measurement outcomes of H (the energy) and what are the associated resulting states after measuring H .

Solution

First write down the matrix form of H in the $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$ basis

$$H = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (65)$$

Using the method demonstrated in the previous problem, we can construct the projection operators

$$P(H = 1) = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}, \quad P(H = -3) = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (66)$$

The initial state is

$$|\psi_0\rangle = |\uparrow\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}. \quad (67)$$

By measuring H : the probability to obtain $H = 1$ is $\langle\psi_0| P(H = 1) |\psi_0\rangle = 1/2$, which ends up with

$$|\psi_1\rangle = \frac{P(H = 1) |\psi_0\rangle}{\langle\psi_0| P(H = 1) |\psi_0\rangle^{1/2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle); \quad (68)$$

the probability to obtain $H = -3$ is $\langle\psi_0| P(H = -3) |\psi_0\rangle = 1/2$, which ends up with

$$|\psi_1\rangle = \frac{P(H = -3) |\psi_0\rangle}{\langle\psi_0| P(H = -3) |\psi_0\rangle^{1/2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \quad (69)$$

■ Partial Trace

■ Applying the Formula

Given the arrangement of the basis $|ij\rangle = |i\rangle_A \otimes |j\rangle_B$, and the operator

$$X = \sum_{ijkl} |ij\rangle X_{ij,kl} \langle kl|. \quad (70)$$

The partial traces are given by

$$\begin{aligned} \text{Tr}_A X &= \sum_{jl} |j\rangle \left(\sum_i X_{ij,il} \right) \langle l|, \\ \text{Tr}_B X &= \sum_{ik} |i\rangle \left(\sum_j X_{ij,kj} \right) \langle k|. \end{aligned} \quad (71)$$

**Exc
20**

Given the following operator in a two-qubit system

$$X = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{pmatrix},$$

calculate the partial traces $\text{Tr}_A X$ and $\text{Tr}_B X$.

Solution

$$\text{Tr}_A X = \begin{pmatrix} \text{Tr} \begin{pmatrix} 1 & 3 \\ 9 & 11 \end{pmatrix} & \text{Tr} \begin{pmatrix} 2 & 4 \\ 10 & 12 \end{pmatrix} \\ \text{Tr} \begin{pmatrix} 5 & 7 \\ 13 & 15 \end{pmatrix} & \text{Tr} \begin{pmatrix} 6 & 8 \\ 14 & 16 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 12 & 14 \\ 20 & 22 \end{pmatrix}. \quad (72)$$

$$\text{Tr}_B X = \begin{pmatrix} \text{Tr} \begin{pmatrix} 1 & 2 \\ 5 & 6 \end{pmatrix} & \text{Tr} \begin{pmatrix} 3 & 4 \\ 7 & 8 \end{pmatrix} \\ \text{Tr} \begin{pmatrix} 9 & 10 \\ 13 & 14 \end{pmatrix} & \text{Tr} \begin{pmatrix} 11 & 12 \\ 15 & 16 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 7 & 11 \\ 23 & 27 \end{pmatrix}. \quad (73)$$

■ Tensor Product Rules

If $X = X_A \otimes X_B$,

$$\text{Tr}_A X = (\text{Tr } X_A) X_B,$$

$$\text{Tr}_B X = (\text{Tr } X_B) X_A.$$

(74)

**Exc
21**

Given the following density matrix

$$\rho = \frac{1}{4} (\mathbb{1} + \sigma_A \cdot \sigma_B),$$

calculate $\text{Tr}_B \rho$.

Solution

$$\rho = \frac{1}{4} (\mathbb{1} + \sigma_A \cdot \sigma_B) = \frac{1}{4} (\mathbb{1}_A \otimes \mathbb{1}_B + \sigma_A^x \otimes \sigma_B^x + \sigma_A^y \otimes \sigma_B^y + \sigma_A^z \otimes \sigma_B^z). \quad (75)$$

Therefore

$$\begin{aligned} \text{Tr}_B \rho &= \frac{1}{4} \text{Tr}_B (\mathbb{1}_A \otimes \mathbb{1}_B + \sigma_A^x \otimes \sigma_B^x + \sigma_A^y \otimes \sigma_B^y + \sigma_A^z \otimes \sigma_B^z) \\ &= \frac{1}{4} (\text{Tr}_B (\mathbb{1}_A \otimes \mathbb{1}_B) + \text{Tr}_B (\sigma_A^x \otimes \sigma_B^x) + \text{Tr}_B (\sigma_A^y \otimes \sigma_B^y) + \text{Tr}_B (\sigma_A^z \otimes \sigma_B^z)) \\ &= \frac{1}{4} (\mathbb{1}_A \text{Tr}(\mathbb{1}_B) + \sigma_A^x \text{Tr}(\sigma_B^x) + \sigma_A^y \text{Tr}(\sigma_B^y) + \sigma_A^z \text{Tr}(\sigma_B^z)) \\ &= \frac{1}{4} (\mathbb{1}_A \times 2 + \sigma_A^x \times 0 + \sigma_A^y \times 0 + \sigma_A^z \times 0) \end{aligned} \quad (76)$$

$$= \frac{1}{2} \mathbb{1}_A \simeq \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

State and Operator

■ State Representation

Given a complete set of orthonormal basis $\{|1\rangle, |2\rangle, |3\rangle, \dots\}$, a quantum state can be represented as a state vector by collecting coefficients in front of each basis state as vector components

$$|\psi\rangle = \psi_1 |1\rangle + \psi_2 |2\rangle + \psi_3 |3\rangle + \dots$$

$$\rightarrow |\psi\rangle \simeq \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \end{pmatrix}. \quad (77)$$

■ Two-Qubit State

**Exc
22**

Consider a two-qubit system spanned by the basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, represent the EPR state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ as a state vector.

Solution

Spell out the state as a linear combination of basis states

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = 0|\uparrow\uparrow\rangle + \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle + \left(-\frac{1}{\sqrt{2}}\right)|\downarrow\uparrow\rangle + 0|\downarrow\downarrow\rangle, \quad (78)$$

then collect the coefficients into the state vector

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \simeq \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}. \quad (79)$$

- Prepend 0 as the coefficient to the basis states that has not appeared.
- Always collect the coefficients following the same order of the basis state.

■ Operator Representation

Given a complete set of orthonormal basis $\{|1\rangle, |2\rangle, |3\rangle, \dots\}$, a quantum operator can be represented as a matrix, such that the i th row j th column matrix element is the coefficient in front of

$|i\rangle\langle j|$.

$$\begin{aligned}
 M &= \sum_{i,j} M_{ij} |i\rangle\langle j| \\
 &\rightarrow M \simeq \begin{pmatrix} M_{11} & M_{12} & \cdots \\ M_{21} & M_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}.
 \end{aligned} \tag{80}$$

■ Permutation Operator

Exc 23 A permutation operator A acts on the basis states $\{|\diamond\rangle, |\clubsuit\rangle, |\heartsuit\rangle, |\spadesuit\rangle\}$ as $A|\diamond\rangle = |\heartsuit\rangle$, $A|\heartsuit\rangle = |\diamond\rangle$, $A|\clubsuit\rangle = |\spadesuit\rangle$, $A|\spadesuit\rangle = |\clubsuit\rangle$. Represent A as matrix in the given basis.

Solution 1

The basis states are represented as the following vectors

$$|\diamond\rangle \simeq \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |\clubsuit\rangle \simeq \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |\heartsuit\rangle \simeq \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |\spadesuit\rangle \simeq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{81}$$

The operator A acting on the four states must be represented as a 4×4 matrix. Suppose the matrix takes the form of

$$A \simeq \begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{pmatrix}. \tag{82}$$

The first rule $A|\diamond\rangle = |\heartsuit\rangle$ implies

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} A_{11} \\ A_{21} \\ A_{31} \\ A_{41} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}. \tag{83}$$

So $A_{11} = 0$, $A_{21} = 0$, $A_{31} = 1$, $A_{41} = 0$, and the matrix representation becomes

$$A \simeq \begin{pmatrix} 0 & A_{12} & A_{13} & A_{14} \\ 0 & A_{22} & A_{23} & A_{24} \\ 1 & A_{32} & A_{33} & A_{34} \\ 0 & A_{42} & A_{43} & A_{44} \end{pmatrix}. \tag{84}$$

Continue with the second rule $A|\heartsuit\rangle = |\diamond\rangle$, which implies

$$\begin{pmatrix} 0 & A_{12} & A_{13} & A_{14} \\ 0 & A_{22} & A_{23} & A_{24} \\ 1 & A_{32} & A_{33} & A_{34} \\ 0 & A_{42} & A_{43} & A_{44} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} A_{13} \\ A_{23} \\ A_{33} \\ A_{43} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (85)$$

thus the matrix representation becomes

$$A \simeq \begin{pmatrix} 0 & A_{12} & 1 & A_{14} \\ 0 & A_{22} & 0 & A_{24} \\ 1 & A_{32} & 0 & A_{34} \\ 0 & A_{42} & 0 & A_{44} \end{pmatrix}. \quad (86)$$

Continue with the second rule $A|\heartsuit\rangle = |\diamond\rangle$, which implies

$$\begin{pmatrix} 0 & A_{12} & A_{13} & A_{14} \\ 0 & A_{22} & A_{23} & A_{24} \\ 1 & A_{32} & A_{33} & A_{34} \\ 0 & A_{42} & A_{43} & A_{44} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} A_{13} \\ A_{23} \\ A_{33} \\ A_{43} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (87)$$

thus the matrix representation becomes

$$A \simeq \begin{pmatrix} 0 & A_{12} & 1 & A_{14} \\ 0 & A_{22} & 0 & A_{24} \\ 1 & A_{32} & 0 & A_{34} \\ 0 & A_{42} & 0 & A_{44} \end{pmatrix}. \quad (88)$$

Continue with the third rule $A|\clubsuit\rangle = |\spadesuit\rangle$, we will determine the 2nd column

$$A \simeq \begin{pmatrix} 0 & 0 & 1 & A_{14} \\ 0 & 0 & 0 & A_{24} \\ 1 & 0 & 0 & A_{34} \\ 0 & 1 & 0 & A_{44} \end{pmatrix}. \quad (89)$$

Continue with the last rule $A|\spadesuit\rangle = |\clubsuit\rangle$, we will determine the 4th column

$$A \simeq \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (90)$$

Solution 2

Make a table to keep track of which state goes to which state under the action of operator A

out\in	$ \diamond\rangle$	$ \clubsuit\rangle$	$ \heartsuit\rangle$	$ \spadesuit\rangle$
$ \diamond\rangle$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
$ \clubsuit\rangle$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
$ \heartsuit\rangle$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
$ \spadesuit\rangle$	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

(91)

The first rule $A|\diamond\rangle = |\heartsuit\rangle$ states that the operator A takes $|\diamond\rangle$ to $|\heartsuit\rangle \rightarrow$ we should put a 1 at the $|\heartsuit\rangle$'s

row and $|\diamond\rangle$'s column

out\in	$ \diamond\rangle$	$ \clubsuit\rangle$	$ \heartsuit\rangle$	$ \spadesuit\rangle$
$ \diamond\rangle$	\square	\square	\square	\square
$ \clubsuit\rangle$	\square	\square	\square	\square
$ \heartsuit\rangle$	1	\square	\square	\square
$ \spadesuit\rangle$	\square	\square	\square	\square

(92)

For the second rule $A|\heartsuit\rangle = |\diamond\rangle$, we put

out\in	$ \diamond\rangle$	$ \clubsuit\rangle$	$ \heartsuit\rangle$	$ \spadesuit\rangle$
$ \diamond\rangle$	\square	\square	1	\square
$ \clubsuit\rangle$	\square	\square	\square	\square
$ \heartsuit\rangle$	1	\square	\square	\square
$ \spadesuit\rangle$	\square	\square	\square	\square

(93)

For the third rule $A|\spadesuit\rangle = |\spadesuit\rangle$, we put

out\in	$ \diamond\rangle$	$ \clubsuit\rangle$	$ \heartsuit\rangle$	$ \spadesuit\rangle$
$ \diamond\rangle$	\square	\square	1	\square
$ \clubsuit\rangle$	\square	\square	\square	\square
$ \heartsuit\rangle$	1	\square	\square	\square
$ \spadesuit\rangle$	\square	1	\square	\square

(94)

For the fourth rule $A|\spadesuit\rangle = |\clubsuit\rangle$, we put

out\in	$ \diamond\rangle$	$ \clubsuit\rangle$	$ \heartsuit\rangle$	$ \spadesuit\rangle$
$ \diamond\rangle$	\square	\square	1	\square
$ \clubsuit\rangle$	\square	\square	\square	1
$ \heartsuit\rangle$	1	\square	\square	\square
$ \spadesuit\rangle$	\square	1	\square	\square

(95)

Pad the empty elements with 0, the matrix representation reads

$$A \simeq \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (96)$$

Solution 3

The fact that the operator A can take $|\diamond\rangle$ to $|\heartsuit\rangle$ implies that A contains a term $|\heartsuit\rangle\langle\diamond|$ (reads take \diamond to \heartsuit) to implement this operation. Thus the rules implies that A should be written as

$$A = |\heartsuit\rangle\langle\diamond| + |\diamond\rangle\langle\heartsuit| + |\spadesuit\rangle\langle\clubsuit| + |\clubsuit\rangle\langle\spadesuit|. \quad (97)$$

According to Eq. (80), we can collect the coefficients to form the matrix representation

$$A \simeq \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (98)$$

■ Hadamard Gate (I)

Exc 24 Hadamard gate U_H is a single-qubit gate that takes $|\rightarrow\rangle$ to $|\uparrow\rangle$ and takes $|\leftarrow\rangle$ to $|\downarrow\rangle$. Represent U_H in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis.

Solution

Note that

$$|\rightarrow\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}, |\leftarrow\rangle = \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}}. \quad (99)$$

The Hadamard gate operation can be denoted as

$$\begin{aligned} U_H &= |\uparrow\rangle\langle\rightarrow| + |\downarrow\rangle\langle\leftarrow| \\ &= |\uparrow\rangle \frac{\langle\uparrow| + \langle\downarrow|}{\sqrt{2}} + |\downarrow\rangle \frac{\langle\uparrow| - \langle\downarrow|}{\sqrt{2}} \\ &= \frac{|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|}{\sqrt{2}}, \end{aligned} \quad (100)$$

therefore the matrix representation is

$$U_H \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (101)$$

■ Basis Transformation

The same state (operator) can have many different vector (matrix) representations depending on the choice of basis. Basis transformation take the representation in one set of basis to another. It is always implemented by a unitary operator U , under which a state transforms as

$$|\psi\rangle \rightarrow U |\psi\rangle, \quad (102)$$

and an operator transforms as

$$M \rightarrow U M U^\dagger. \quad (103)$$

■ Hadamard Gate (II)

**Exc
25**

Hadamard gate $U_H = |\uparrow\rangle\langle\rightarrow| + |\downarrow\rangle\langle\leftarrow|$ performs basis transformation from σ^x eigen basis to σ^z eigen basis.

- (i) How does the states $|\rightarrow\rangle$ and $|\leftarrow\rangle$ transforms under U_H .
(ii) How does the operator σ^x transforms under U_H

Solution 1

Using Dirac notation

- (i) Acting on state

$$\begin{aligned}
 U_H |\rightarrow\rangle &= (|\uparrow\rangle\langle\rightarrow| + |\downarrow\rangle\langle\leftarrow|) |\rightarrow\rangle \\
 &= |\uparrow\rangle\langle\rightarrow|\rightarrow\rangle + |\downarrow\rangle\langle\leftarrow|\rightarrow\rangle \\
 &= |\uparrow\rangle 1 + |\downarrow\rangle 0 \\
 &= |\uparrow\rangle.
 \end{aligned} \tag{104}$$

Similarly $U_H |\leftarrow\rangle = |\downarrow\rangle$.

- (ii) Acting on the operator

$$\begin{aligned}
 U_H \sigma^x U_H^\dagger &= (|\uparrow\rangle\langle\rightarrow| + |\downarrow\rangle\langle\leftarrow|) (|\rightarrow\rangle\langle\rightarrow| - |\leftarrow\rangle\langle\leftarrow|) (|\rightarrow\rangle\langle\uparrow| + |\leftarrow\rangle\langle\downarrow|) \\
 &= (|\uparrow\rangle\langle\rightarrow|\rightarrow\rangle\langle\rightarrow| - |\uparrow\rangle\langle\rightarrow|\leftarrow\rangle\langle\leftarrow| + |\downarrow\rangle\langle\leftarrow|\rightarrow\rangle\langle\rightarrow| - |\downarrow\rangle\langle\leftarrow|\leftarrow\rangle\langle\leftarrow|) (|\rightarrow\rangle\langle\uparrow| + |\leftarrow\rangle\langle\downarrow|) \\
 &= (|\uparrow\rangle\langle\rightarrow| - |\downarrow\rangle\langle\leftarrow|) (|\rightarrow\rangle\langle\uparrow| + |\leftarrow\rangle\langle\downarrow|) \\
 &= |\uparrow\rangle\langle\rightarrow|\rightarrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\rightarrow|\leftarrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\leftarrow|\rightarrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\leftarrow|\leftarrow\rangle\langle\downarrow| \\
 &= |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow| \\
 &= \sigma^z.
 \end{aligned} \tag{105}$$

Solution 2

Using vector / matrix representation in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis.

- Note that even though U_H implements basis transformation, when representing states and operators, one must still stick to a single choice of basis (e.g. σ^z eigen basis) for all representations.

$$\begin{aligned}
 U_H &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \\
 |\rightarrow\rangle &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\leftarrow\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \\
 |\uparrow\rangle &\simeq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle \simeq \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \\
 \sigma^x &\simeq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^z \simeq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
 \end{aligned} \tag{106}$$

- (i) Acting on state

$$\begin{aligned}
U_H |\rightarrow\rangle &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \simeq |\uparrow\rangle, \\
U_H |\rightarrow\rangle &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \simeq |\downarrow\rangle.
\end{aligned} \tag{107}$$

(ii) Acting on the operator

$$\begin{aligned}
U_H \sigma^x U_H^\dagger &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \simeq \sigma^z.
\end{aligned} \tag{108}$$

- One can see that U_H is actually the unitary transformation that diagonalize the σ^x matrix.

Evolution and Measurement

■ Time Evolution

Time evolution of a quantum system is described by the Schrödinger equation (set $\hbar = 1$)

$$i \partial_t |\psi(t)\rangle = H |\psi(t)\rangle. \tag{109}$$

In the case that the Hamiltonian H is time independent, we can use H to generate the unitary time evolution operator

$$U(t) = e^{-i H t}, \tag{110}$$

and then use $U(t)$

- to evolve a state $|\psi(0)\rangle$ in time (Schrödinger picture)

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle, \tag{111}$$

- or to evolve a density matrix $\rho(0)$ in time (Schrödinger picture)

$$\rho(t) = U(t) \rho(0) U(t)^\dagger. \tag{112}$$

■ Evolution of a Single-Qubit System

Exc 26 Calculate the time evolution of a single-qubit density matrix $\rho(0) = \frac{1}{2} (\mathbf{1} + \mathbf{m} \cdot \boldsymbol{\sigma})$ under the Hamiltonian $H = \mathbf{h} \cdot \boldsymbol{\sigma}$

Solution

First calculate the time evolution operator [Using Eq. (41)]

$$\begin{aligned}
U(t) &= e^{-iHt} = \exp(-i\mathbf{h} \cdot \boldsymbol{\sigma} t) = \exp(-i\hat{\mathbf{h}} \cdot \boldsymbol{\sigma} |\mathbf{h}| t) \\
&= \cos(|\mathbf{h}| t) \mathbb{1} - i \sin(|\mathbf{h}| t) \hat{\mathbf{h}} \cdot \boldsymbol{\sigma},
\end{aligned} \tag{113}$$

where $|\mathbf{h}| = \sqrt{\mathbf{h} \cdot \mathbf{h}}$ is the norm of the vector \mathbf{h} , and $\hat{\mathbf{h}} = \mathbf{h}/|\mathbf{h}|$ is the direction (unit vector).

Then apply the unitary evolution operator

$$\begin{aligned}
\rho(t) &= U(t) \rho(0) U(t)^\dagger \\
&= \left(\cos(|\mathbf{h}| t) \mathbb{1} - i \sin(|\mathbf{h}| t) \hat{\mathbf{h}} \cdot \boldsymbol{\sigma} \right) \frac{1}{2} (\mathbb{1} + \mathbf{m} \cdot \boldsymbol{\sigma}) \left(\cos(|\mathbf{h}| t) \mathbb{1} + i \sin(|\mathbf{h}| t) \hat{\mathbf{h}} \cdot \boldsymbol{\sigma} \right).
\end{aligned} \tag{114}$$

In $\frac{1}{2} (\mathbb{1} + \mathbf{m} \cdot \boldsymbol{\sigma})$, the identity operator $\mathbb{1}$ will not be transformed by the unitary, we can focus on how $\mathbf{m} \cdot \boldsymbol{\sigma}$ is transformed.

$$\begin{aligned}
&\left(\cos(|\mathbf{h}| t) \mathbb{1} - i \sin(|\mathbf{h}| t) \hat{\mathbf{h}} \cdot \boldsymbol{\sigma} \right) \mathbf{m} \cdot \boldsymbol{\sigma} \left(\cos(|\mathbf{h}| t) \mathbb{1} + i \sin(|\mathbf{h}| t) \hat{\mathbf{h}} \cdot \boldsymbol{\sigma} \right) \\
&= \cos^2(|\mathbf{h}| t) \mathbf{m} \cdot \boldsymbol{\sigma} - i \sin(|\mathbf{h}| t) \cos(|\mathbf{h}| t) \left[\hat{\mathbf{h}} \cdot \boldsymbol{\sigma}, \mathbf{m} \cdot \boldsymbol{\sigma} \right] + \sin^2(|\mathbf{h}| t) \hat{\mathbf{h}} \cdot \boldsymbol{\sigma} \mathbf{m} \cdot \boldsymbol{\sigma} \hat{\mathbf{h}} \cdot \boldsymbol{\sigma} \\
&= \cos^2(|\mathbf{h}| t) \mathbf{m} \cdot \boldsymbol{\sigma} + 2 \sin(|\mathbf{h}| t) \cos(|\mathbf{h}| t) (\hat{\mathbf{h}} \times \mathbf{m}) \cdot \boldsymbol{\sigma} + \sin^2(|\mathbf{h}| t) (2 \hat{\mathbf{h}} \cdot \mathbf{m} \hat{\mathbf{h}} \cdot \boldsymbol{\sigma} - \mathbf{m} \cdot \boldsymbol{\sigma}) \\
&= \cos(2|\mathbf{h}| t) \mathbf{m} \cdot \boldsymbol{\sigma} + \sin(2|\mathbf{h}| t) \mathbf{m} \cdot (\hat{\mathbf{h}} \times \boldsymbol{\sigma}) + (1 - \cos(2|\mathbf{h}| t)) \hat{\mathbf{h}} \cdot \mathbf{m} \hat{\mathbf{h}} \cdot \boldsymbol{\sigma}.
\end{aligned} \tag{115}$$

Therefore

$$\rho(t) = \frac{1}{2} \left(\mathbb{1} + \cos(2|\mathbf{h}| t) \mathbf{m} \cdot \boldsymbol{\sigma} + \sin(2|\mathbf{h}| t) \mathbf{m} \cdot (\hat{\mathbf{h}} \times \boldsymbol{\sigma}) + (1 - \cos(2|\mathbf{h}| t)) \hat{\mathbf{h}} \cdot \mathbf{m} \hat{\mathbf{h}} \cdot \boldsymbol{\sigma} \right). \tag{116}$$

■ Evolution of a Two-Qubit System

Exc
27

Consider a two-qubit state $|\psi(0)\rangle = |\uparrow\downarrow\rangle$ evolved under the Hamiltonian $H = |\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow|$, write down the state $|\psi(t)\rangle$ as a function of time.

Solution 1

Using the full basis representation.

A two-qubit system is spanned by the four basis states $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$. Represent the initial state and the Hamiltonian in this set of basis

$$|\psi(0)\rangle = |\uparrow\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \tag{117}$$

$$H = |\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

H is independent of time, we can compute the time-evolution operator (following the similar approach in (Exc. 13) or use *Mathematica*)

$$U(t) = e^{-iHt} \simeq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos t & -i \sin t & 0 \\ 0 & -i \sin t & \cos t & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (118)$$

```
MatrixExp[-i {{0, 0, 0, 0}, {0, 0, 1, 0}, {0, 1, 0, 0}, {0, 0, 0, 0}} t]
{{1, 0, 0, 0}, {0, Cos[t], -i Sin[t], 0}, {0, -i Sin[t], Cos[t], 0}, {0, 0, 0, 1}}
```

Apply the time evolution operator to the initial state

$$\begin{aligned} |\psi(t)\rangle &= U(t) |\psi(0)\rangle \simeq \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos t & -i \sin t & 0 \\ 0 & -i \sin t & \cos t & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \cos t \\ -i \sin t \\ 0 \end{pmatrix} \\ &\simeq \cos t |\uparrow\downarrow\rangle - i \sin t |\downarrow\uparrow\rangle. \end{aligned} \quad (119)$$

As a check, by setting $t = 0$, the result indeed reduces to $|\psi(0)\rangle$.

Solution 2

Using representation only in the relevant subspace.

- Notice that both the initial state and the Hamiltonian only involves the basis states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$. So $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ are the *relevant* set of basis. The other states like $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are *irrelevant* to our problem.

In the relevant subspace spanned by the basis $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$, the initial state and the Hamiltonian are represented as

$$|\psi(0)\rangle = |\uparrow\downarrow\rangle \simeq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad (120)$$

$$H = |\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow| \simeq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma^x.$$

H is independent of time, we can compute the time-evolution operator

$$\begin{aligned} U(t) &= e^{-iHt} \simeq e^{-i\sigma^x t} = \cos t \mathbb{1} - i \sin t \sigma^x \\ &= \begin{pmatrix} \cos t & -i \sin t \\ -i \sin t & \cos t \end{pmatrix}. \end{aligned} \quad (121)$$

Apply the time evolution operator to the initial state

$$\begin{aligned} |\psi(t)\rangle &= U(t) |\psi(0)\rangle \simeq \begin{pmatrix} \cos t & -i \sin t \\ -i \sin t & \cos t \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos t \\ -i \sin t \end{pmatrix} \\ &\simeq \cos t |\uparrow\downarrow\rangle - i \sin t |\downarrow\uparrow\rangle. \end{aligned} \quad (122)$$

As a check, by setting $t = 0$, the result indeed reduces to $|\psi(0)\rangle$.

■ Measurement

Measurement is implemented by projection operator. Each projection operator $P(L = \lambda)$ is associate with the event of measuring L and obtaining the outcome λ . The probability for the event $L = \lambda$ to happen is given by

- for pure state

$$p(L = \lambda) = \langle \psi | P(L = \lambda) | \psi \rangle, \quad (123)$$

- for mixed state

$$p(L = \lambda) = \text{Tr } \rho P(L = \lambda). \quad (124)$$

Conditioned on the measurement outcome, the state will collapse to

- for pure state

$$|\psi\rangle \xrightarrow{\text{measure } L, \text{ get } \lambda} \frac{P(L = \lambda) |\psi\rangle}{p(L = \lambda)^{1/2}}, \quad (125)$$

- for mixed state

$$\rho \xrightarrow{\text{measure } L, \text{ get } \lambda} \frac{P(L = \lambda) \rho P(L = \lambda)}{p(L = \lambda)}. \quad (126)$$

■ Single-Qubit Measurement

Exc
28

Consider a single qubit state $|\psi\rangle = \cos \alpha |\uparrow\rangle + \sin \alpha |\downarrow\rangle$. Measure σ^z

- What are the possible measurement outcomes?
- What are the probabilities associated to the possible outcomes?
- For each measurement outcome, what post-measurement state will the system collapse to?

Solution

(i) The possible measurement outcomes of an observable σ^z are the eigenvalues of the operator σ^z , which are ± 1 .

(ii) Construct the projection operators associated with each outcome [use Eq. (62)]

$$P(\sigma^z = \pm 1) = \frac{1 \pm \sigma^z}{2}. \quad (127)$$

The measurement outcome probability is given by

$$\begin{aligned} p(\sigma^z = \pm 1) &= \langle \psi | P(\sigma^z = \pm 1) | \psi \rangle \\ &= (\cos \alpha \langle \uparrow | + \sin \alpha \langle \downarrow |) \frac{1 \pm \sigma^z}{2} (\cos \alpha |\uparrow\rangle + \sin \alpha |\downarrow\rangle) \\ &= \frac{1}{2} (1 \pm (\cos^2 \alpha - \sin^2 \alpha)). \end{aligned} \quad (128)$$

Or more explicitly

$$\begin{aligned} p(\sigma^z = +1) &= \cos^2 \alpha, \\ p(\sigma^z = -1) &= \sin^2 \alpha. \end{aligned} \tag{129}$$

(iii) The post-measurement state is given by

$$\begin{aligned} |\psi\rangle &\xrightarrow{\sigma^z=+1} \frac{P(\sigma^z = +1) |\psi\rangle}{p(\sigma^z = +1)^{1/2}} \\ &= \frac{1}{\cos \alpha} \frac{1 + \sigma^z}{2} (\cos \alpha |\uparrow\rangle + \sin \alpha |\downarrow\rangle) \\ &= \frac{1}{\cos \alpha} \left(\cos \alpha \frac{1 + \sigma^z}{2} |\uparrow\rangle + \sin \alpha \frac{1 + \sigma^z}{2} |\downarrow\rangle \right) \\ &= \frac{1}{\cos \alpha} \left(\cos \alpha \frac{1 + 1}{2} |\uparrow\rangle + \sin \alpha \frac{1 - 1}{2} |\downarrow\rangle \right) \\ &= \frac{1}{\cos \alpha} \cos \alpha |\uparrow\rangle \\ &= |\uparrow\rangle \end{aligned} \tag{130}$$

Similarly

$$|\psi\rangle \xrightarrow{\sigma^z=-1} \frac{P(\sigma^z = -1) |\psi\rangle}{p(\sigma^z = -1)^{1/2}} = |\downarrow\rangle. \tag{131}$$

■ Measurement with Degenerated Subspace

**Exc
29**

Consider a quantum state $|\psi\rangle = \frac{1}{\sqrt{3}} (|1\rangle + |2\rangle + |3\rangle)$, measure the observable $L = (|1\rangle - |2\rangle)(\langle 1| - \langle 2|)$.
 (i) What are the possible measurement outcomes?
 (ii) If the measurement outcome is $L = 0$, which state will the system collapse to?

Solution

Represent the state and operator in the basis $\{|1\rangle, |2\rangle, |3\rangle\}$.

$$\begin{aligned} |\psi\rangle &= \frac{1}{\sqrt{3}} (|1\rangle + |2\rangle + |3\rangle) \simeq \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \\ L &= (|1\rangle + |2\rangle)(\langle 1| + \langle 2|) \simeq \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned} \tag{132}$$

Using the techniques of Eq. (8) and Eq. (9) to diagonalize L . We find three eigenvalues: 1 ± 1 and 0, with the corresponding eigen states

$$|1+1\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \quad |1-1\rangle \simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad |0\rangle \simeq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (133)$$

(i) The possible measurement outcomes are the eigenvalues of L , which are 2 and 0.

(ii) Construct the projection operator of $L = 0$, by definition Eq. (53),

$$\begin{aligned} P(L = 0) &= \sum_i |\lambda_i\rangle \delta(\lambda_i - 0) \langle \lambda_i| \\ &= |1+1\rangle \delta(2-0) \langle 1+1| + |1-1\rangle \delta(0-0) \langle 1-1| + |0\rangle \delta(0-0) \langle 0| \\ &= |1-1\rangle \langle 1-1| + |0\rangle \langle 0| \\ &\simeq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2}} (1 \quad 1 \quad 0) + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} (0 \quad 0 \quad 1) \\ &= \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (134)$$

The probability for $L = 0$ to occur on the state $|\psi\rangle$ is

$$\begin{aligned} p(L = 0) &= \langle \psi | P(L = 0) | \psi \rangle \\ &\simeq \frac{1}{\sqrt{3}} (1 \quad 1 \quad 1) \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \\ &= \frac{1}{3} (1 \quad 1 \quad 1) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \\ &= 1. \end{aligned} \quad (135)$$

According to Eq. (125), if the measurement outcome is $L = 0$, the post-measurement state is

$$\begin{aligned} |\psi\rangle &\xrightarrow{L=0} \frac{P(L=0) |\psi\rangle}{p(L=0)^{1/2}} \\ &\simeq \begin{pmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \\ &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \simeq |\psi\rangle, \end{aligned} \quad (136)$$

i.e. after measurement the state remains the same (because $|\psi\rangle$ happens to be an eigenstate of L of eigenvalue 0).

■ Entanglement by Measurement

**Exc
30**

Consider a two-qubit system describe by a product state $|\psi\rangle = \frac{1}{2}(|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle)$, measure $L = |\uparrow\uparrow\rangle\langle\downarrow\downarrow| + |\downarrow\downarrow\rangle\langle\uparrow\uparrow|$, suppose the outcome $L = +1$ is obtained, what is the post-measurement state that the system collapses to?

Solution

Choose the basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$,

$$\begin{aligned} |\psi\rangle &= \frac{1}{2}(|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle) \\ &= \frac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle) \\ &\doteq \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \end{aligned} \tag{137}$$

$$L \doteq \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Construct the projection operator

$$P(L = +1) = \frac{\mathbb{1} + L}{2} \doteq \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}. \tag{138}$$

The probability for $L = +1$ to occur is

$$\begin{aligned} p(L = +1) &= \langle\psi| P(L = +1) |\psi\rangle \\ &\doteq \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \\ &= \frac{1}{2}. \end{aligned} \tag{139}$$

The state will collapse to

$$\begin{aligned}
|\psi\rangle &\xrightarrow{L=+1} \frac{P(L=+1)|\psi\rangle}{p(L=+1)^{1/2}} \\
&\cong \frac{1}{\sqrt{1/2}} \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \\
&\cong \frac{|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle}{\sqrt{2}},
\end{aligned}$$

which is an entangled state. This shows that measurement can create entanglement in quantum systems.