

First of all this is based on the book Using Mathematica for quantum mechanics by Roman Schmied, this is simply exercise 2.1

We describe a spin-1/2 system in the basis \mathcal{B} containing the two states

$$\begin{aligned} |\uparrow_{\vartheta, \varphi}\rangle &= \cos\left(\frac{\vartheta}{2}\right) |\uparrow\rangle + e^{i\varphi} \sin\left(\frac{\vartheta}{2}\right) |\downarrow\rangle \\ |\downarrow_{\vartheta, \varphi}\rangle &= -e^{-i\varphi} \sin\left(\frac{\vartheta}{2}\right) |\uparrow\rangle + \cos\left(\frac{\vartheta}{2}\right) |\downarrow\rangle \end{aligned} \quad (2.8)$$

1. Show that the basis $\mathcal{B} = \{|\uparrow_{\vartheta, \varphi}\rangle, |\downarrow_{\vartheta, \varphi}\rangle\}$ is orthonormal.
2. Show that the basis \mathcal{B} is complete: $|\uparrow_{\vartheta, \varphi}\rangle\langle\uparrow_{\vartheta, \varphi}| + |\downarrow_{\vartheta, \varphi}\rangle\langle\downarrow_{\vartheta, \varphi}| = \mathbb{1}$.
3. Express the states $|\uparrow\rangle$ and $|\downarrow\rangle$ as vectors in the basis \mathcal{B} .
4. Express the Pauli operators $\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z$ as matrices in the basis \mathcal{B} .
5. Show that $|\uparrow_{\vartheta, \varphi}\rangle$ and $|\downarrow_{\vartheta, \varphi}\rangle$ are eigenvectors of $\hat{\sigma}(\vartheta, \varphi) = \hat{\sigma}_x \sin(\vartheta) \cos(\varphi) + \hat{\sigma}_y \sin(\vartheta) \sin(\varphi) + \hat{\sigma}_z \cos(\vartheta)$. What are the eigenvalues?

We start by defining the up and down basis

```
In[ ]:= up = {Cos[ϑ / 2], Exp[I ϕ] Sin[ϑ / 2]}
Out[ ]:= {Cos[ϑ / 2], Exp[I ϕ] Sin[ϑ / 2]}

In[ ]:= MatrixForm[%]
Out[ ]//MatrixForm=

$$\begin{pmatrix} \cos\left[\frac{\vartheta}{2}\right] \\ e^{i\varphi} \sin\left[\frac{\vartheta}{2}\right] \end{pmatrix}$$


In[ ]:= down = {-Exp[-I ϕ] Sin[ϑ / 2], Cos[ϑ / 2]}
MatrixForm[down[ϕ, ϑ]]
Out[ ]:= {-Exp[-I ϕ] Sin[ϑ / 2], Cos[ϑ / 2]}

Out[ ]//MatrixForm=

$$\left\{-e^{-i\varphi} \sin\left[\frac{\vartheta}{2}\right], \cos\left[\frac{\vartheta}{2}\right]\right\}[\varphi, \vartheta]$$

```

To show that this basis is orthonormal, we just do the internal product and we expect $\langle i | j \rangle = \delta_{ij}$ if it is an orthonormal basis. Note that we do not need to transpose as the Dot function in Mathematica does it for us

```
In[ ]:= ComplexExpand[up. Conjugate[down]]
Out[ ]:= 0
```

Or alternative and way better looking

```
In[ ]:= up. Conjugate[down] // ComplexExpand
```

```
Out[ ]:= 0
```

```
In[ ]:= up. Conjugate[up] // ComplexExpand
```

```
Out[ ]:= Cos[ $\frac{\gamma}{2}$ ]^2 + Sin[ $\frac{\gamma}{2}$ ]^2
```

That's obviously one, here we are in need of the full simplify

```
In[ ]:= up. Conjugate[up] // ComplexExpand // FullSimplify
```

```
Out[ ]:= 1
```

```
In[ ]:= down. Conjugate[down] // ComplexExpand // FullSimplify
```

```
Out[ ]:= 1
```

To show that the basis is complete we need to use the Kronecker product, to construct matrices from ket-bras

```
In[ ]:= upup = KroneckerProduct[up, Conjugate[up]] // ComplexExpand // FullSimplify
```

```
Out[ ]:= {{Cos[ $\frac{\gamma}{2}$ ]^2,  $\frac{1}{2} e^{-i \phi} \sin[\gamma]$ }, { $\frac{1}{2} e^{i \phi} \sin[\gamma]$ , Sin[ $\frac{\gamma}{2}$ ]^2}}
```

```
In[ ]:= downdown = KroneckerProduct[down, Conjugate[down]] // ComplexExpand // FullSimplify
```

```
Out[ ]:= {{Sin[ $\frac{\gamma}{2}$ ]^2,  $-\frac{1}{2} e^{-i \phi} \sin[\gamma]$ }, { $-\frac{1}{2} e^{i \phi} \sin[\gamma]$ , Cos[ $\frac{\gamma}{2}$ ]^2}}
```

```
In[ ]:= upup + downdown // FullSimplify
```

```
Out[ ]:= {{1, 0}, {0, 1}}
```

Now we are asked to express the two vectors that compose our basis in our basis, to to this we simply use $A = \sum_{ij} A_{ij} |i\rangle \langle j|$, where $A_{ij} = \langle i | A | j \rangle$ then

```
In[ ]:= newup = Conjugate[up[[1]]] up + Conjugate[down[[1]]] down // ComplexExpand // FullSimplify
```

```
Out[ ]:= {1, 0}
```

```
In[ ]:= newdown =
```

```
Conjugate[up[[2]]] up + Conjugate[down[[2]]] down // ComplexExpand // FullSimplify
```

```
Out[ ]:= {0, 1}
```

For the next section we are asked to express the Pauli operators as matrices in this basis

```
In[ ]:=  $\sigma_x$  = PauliMatrix[1]
 $\sigma_y$  = PauliMatrix[2]
 $\sigma_z$  = PauliMatrix[3]
```

```
Out[ ]:= {{0, 1}, {1, 0}}
```

```
Out[ ]:= {{0, -i}, {i, 0}}
```

```
Out[ ]:= {{1, 0}, {0, -1}}
```

To express it in our basis we use the fact that the elements of an operator in a basis are $A_{ij} = \langle i | A | j \rangle$

```
In[ ]:= E11[A_] = Conjugate[up].A.up // ComplexExpand // FullSimplify;
E12[A_] = Conjugate[up].A.down // ComplexExpand // FullSimplify;
E21[A_] = Conjugate[down].A.up // ComplexExpand // FullSimplify;
E22[A_] = Conjugate[down].A.down // ComplexExpand // FullSimplify;
newpauli[A_] = {{E11[A], E12[A]}, {E21[A], E22[A]}};
```

We can check that they are the same operator using $A = \sum_{ij} A_{ij} |i\rangle \langle j|$, for example

```
In[ ]:=  $\sigma_x$  = newpauli[ $\sigma_x$ ] // ComplexExpand // FullSimplify;
MatrixForm[ $\sigma_x$ ]
```

```
Out[ ]//MatrixForm=
```

$$\begin{pmatrix} \cos[\phi] \sin[\nu] & e^{-i\phi} (\cos[\nu] \cos[\phi] + i \sin[\phi]) \\ e^{i\phi} (\cos[\nu] \cos[\phi] - i \sin[\phi]) & -\cos[\phi] \sin[\nu] \end{pmatrix}$$

```
In[ ]:=  $\sigma_y$  = newpauli[ $\sigma_y$ ] // ComplexExpand // FullSimplify;
MatrixForm[ $\sigma_y$ ]
```

```
Out[ ]//MatrixForm=
```

$$\begin{pmatrix} \sin[\nu] \sin[\phi] & e^{-i\phi} (-i \cos[\phi] + \cos[\nu] \sin[\phi]) \\ e^{i\phi} (i \cos[\phi] + \cos[\nu] \sin[\phi]) & -\sin[\nu] \sin[\phi] \end{pmatrix}$$

```
In[ ]:=  $\sigma_z$  = newpauli[ $\sigma_z$ ] // ComplexExpand // FullSimplify;
MatrixForm[ $\sigma_z$ ]
```

```
Out[ ]//MatrixForm=
```

$$\begin{pmatrix} \cos[\nu] & -e^{-i\phi} \sin[\nu] \\ -e^{i\phi} \sin[\nu] & -\cos[\nu] \end{pmatrix}$$

Let us see if they are the same using $A = \sum_{ij} A_{ij} |i\rangle \langle j|$

```
In[ ]:= Compare[x_] := x[[1, 1]]  $\times$  KroneckerProduct[up, Conjugate[up]] +
x[[1, 2]]  $\times$  KroneckerProduct[up, Conjugate[down]] +
x[[2, 1]]  $\times$  KroneckerProduct[down, Conjugate[up]] +
x[[2, 2]]  $\times$  KroneckerProduct[down, Conjugate[down]] ;
```

```
In[6]:=  $\sigma_x$  == Compare[ $\sigma_x$ ] // ComplexExpand // FullSimplify
```

```
Out[6]= True
```

```
In[6]:=  $\sigma_y$  == Compare[ $\sigma_y$ ] // ComplexExpand // FullSimplify
```

```
Out[6]= True
```

```
In[6]:=  $\sigma_z$  == Compare[ $\sigma_z$ ] // ComplexExpand // FullSimplify
```

```
Out[6]= True
```

For the Last part we simply write this new operator

```
In[6]:=  $\sigma$  =  $\sigma_x$  Sin[ $\nu$ ] Cos[ $\phi$ ] +  $\sigma_y$  Sin[ $\nu$ ] Sin[ $\phi$ ] +  $\sigma_z$  Cos[ $\nu$ ]
```

```
Out[6]= {{Cos[ $\nu$ ], Cos[ $\phi$ ] Sin[ $\nu$ ] -  $i$  Sin[ $\nu$ ] Sin[ $\phi$ ]}, {Cos[ $\phi$ ] Sin[ $\nu$ ] +  $i$  Sin[ $\nu$ ] Sin[ $\phi$ ], -Cos[ $\nu$ ]}}
```

```
In[6]:=  $\sigma$  // Eigenvalues
```

```
Out[6]= {-1, 1}
```

```
In[6]:=  $\sigma$ .up // ComplexExpand // FullSimplify
```

```
Out[6]= {Cos[ $\frac{\nu}{2}$ ],  $e^{i\phi}$  Sin[ $\frac{\nu}{2}$ ]}
```

```
In[6]:= up ==  $\sigma$ .up // ComplexExpand // FullSimplify
```

```
Out[6]= True
```

```
In[6]:=  $\sigma$ .down // ComplexExpand // FullSimplify
```

```
Out[6]= { $e^{-i\phi}$  Sin[ $\frac{\nu}{2}$ ], -Cos[ $\frac{\nu}{2}$ ]}
```

```
In[6]:= down =  $\sigma$ .down // ComplexExpand // FullSimplify
```

```
Out[6]= { $e^{-i\phi}$  Sin[ $\frac{\nu}{2}$ ], -Cos[ $\frac{\nu}{2}$ ]}
```