```
UH.U // Simplify; UH.U // MatrixForm
```

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

$$\eta = \begin{pmatrix} \eta 1 \\ \eta 2 \\ \eta 3 \\ \eta 4 \\ \eta 5 \end{pmatrix};$$

```
s1 = UH.A1.U // Simplify; s1 // MatrixForm
```

$$\begin{pmatrix} 2+\sqrt{3} & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2-\sqrt{3} \end{pmatrix}$$

```
f1 = Transpose[η].s1.η // FullSimplify
```

$$\left\{\left\{\left(2+\sqrt{3}\right)\eta 1^2 + 3\,\eta 2^2 + 2\,\eta 3^2 + \eta 4^2 - \left(-2+\sqrt{3}\right)\eta 5^2\right\}\right\}$$

```
Det[A1]
```

6

```
K1 = eq1[[1, 1]] eq1[[1, 2]] eq1[[1, 3]] eq1[[1, 4]]
   eq1[[1, 5]] // Simplify
```

6

6. Calculation of the average $\langle\psi|\hat{A}|\psi\rangle$

In order to understand the above discussion, for the sake of clarity, we discuss the fundamental mathematics in detail.

6.1 The average $\langle\psi|\hat{A}|\psi\rangle$ under the original basis $\{|b_i\rangle\}$

We consider the two bases $\{|b_i\rangle, |a_i\rangle\}$, where the new basis $\{|a_i\rangle\}$ is related to the original basis $\{\}|b_i\rangle$ through a unitary operator $\hat{U}$,

$$|a_j\rangle = \hat{U}|b_j\rangle, \qquad |b_j\rangle = \hat{U}^+|a_j\rangle, \qquad \langle b_j| = \langle a_j|\hat{U},$$

with $\hat{U}^+\hat{U} = \hat{1}$. $|a_i\rangle$ is the eigenket of the Hermitian operator $\hat{A}$ with the eigenvalue a_i.

$$\hat{A}|a_i\rangle = a_i|a_i\rangle.$$

Note that

$$\langle b_i|a_j\rangle = \langle b_i|\hat{U}|b_j\rangle = \langle a_i|\hat{U}|a_j\rangle,$$

or

$$\langle a_i|\hat{U}|a_j\rangle = \langle b_i|\hat{U}^+\hat{U}\hat{U}|b_j\rangle = \langle b_i|\hat{U}|b_j\rangle.$$

In other word, the matrix element of $\hat{U}$ is independent of the kind of basis (this is very important property). We also note that

$$\langle a_i|\hat{A}|a_j\rangle = \langle b_i|\hat{U}^+\hat{A}\hat{U}|b_j\rangle = a_i\delta_{ij} \qquad \text{(diagonal matrix)}$$

Here we define the Column matrices for the state $|\psi\rangle$ of the system,

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ . \\ . \\ . \\ \beta_n \end{pmatrix} \qquad \boldsymbol{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ . \\ . \\ . \\ \alpha_n \end{pmatrix} \qquad \text{(matrix form)}$$

with

$$\beta_i = \langle b_i | \psi \rangle, \qquad \alpha_i = \langle a_i | \psi \rangle .$$

We now consider the average over the state $|\psi\rangle$ under the original basis $\{|b_i\rangle\}$.

$$\begin{aligned}
\langle A \rangle &= \langle \psi | \hat{A} | \psi \rangle \\
&= \sum_{i,j} \langle \psi | b_i \rangle \langle b_i | \hat{A} | b_j \rangle \langle b_i | \psi \rangle \\
&= \sum_{i,j} \langle b_i | \psi \rangle^* \langle b_i | \hat{A} | b_j \rangle \langle b_i | \psi \rangle \\
&= \sum_{i,j} \beta_i^* A_{ij} \beta_i \\
&= \begin{pmatrix} \beta_1^* & \beta_2^* & . & . & . & \beta_n^* \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & . & . & . & A_{1n} \\ A_{21} & A_{22} & . & . & . & A_n \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ A_{n1} & A_{n2} & . & . & . & A_{nn} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ . \\ . \\ . \\ \beta_n \end{pmatrix} \\
&= \boldsymbol{\beta}^+ \mathbf{A} \boldsymbol{\beta}
\end{aligned}$$

(matrix form), using the closure relation. The relation between $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$ is obtained as follow.

$$\alpha_i = \langle a_i | \psi \rangle$$
$$= \sum_j \langle a_i | b_j \rangle \langle b_j | \psi \rangle$$
$$= \sum_j \langle a_i | b_j \rangle \beta_j$$
$$= \sum_j \langle b_i | \hat{U}^+ | b_j \rangle \beta_j$$

or

$\boldsymbol{\alpha} = \mathbf{U}^+ \boldsymbol{\beta}$ (matrix form)

since $\langle a_i | = \langle b_i | \hat{U}^+$.

6.2 The average $\langle \psi | \hat{A} | \psi \rangle$ under the new basis $\{|a_i\rangle\}$

Next, we now consider the average under the new basis $\{|a_i\rangle\}$.

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$$
$$= \sum_{i,j} \langle \psi | a_i \rangle \langle a_i | \hat{A} | a_j \rangle \langle a_j | \psi \rangle$$
$$= \sum_{i,j} \langle a_i | \psi \rangle^* \langle a_i | \hat{A} | a_j \rangle \langle a_j | \psi \rangle$$
$$= \sum_{i,j} \alpha_i^* a_i \delta_{ij} \alpha_i$$
$$= \begin{pmatrix} \alpha_1^* & \alpha_2^* & . & . & . & \alpha_n^* \end{pmatrix} \begin{pmatrix} a_1 & 0 & . & . & . & 0 \\ 0 & a_2 & . & . & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & 0 & . & . & . & a_n \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ . \\ . \\ . \\ \alpha_n \end{pmatrix}$$
$$= \sum_{i,j} a_i |\alpha_i|^2$$

6.3 The calculation of the average using Mathematica

(i) Find eigenvalue and eigenkets of matrix ***A*** by using Mathematica

Eigensystem[**A**]

which leads to the eigenvalues a_i and eigenkets, $\left|a_i\right\rangle$. The eigenkets ahould be normalized using the program **Normalize**. When the system is degenerate (the same eigenvalues but different states), further we need to use the program Orthogonize for all eigenkets obtained by doing the process of Eigensystem[**A**]

(ii) Determine the unitary matrix ***U***

Unitary matrix ***U*** is defined as

$$\mathbf{U}=\begin{pmatrix} \langle b_1|a_1\rangle & \langle b_1|a_2\rangle & . & . & . & \langle b_1|a_n\rangle \\ \langle b_2|a_1\rangle & \langle b_2|a_2\rangle & . & . & . & \langle b_2|a_n\rangle \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ \langle b_n|a_1\rangle & \langle b_n|a_2\rangle & . & . & . & \langle b_n|a_n\rangle \end{pmatrix}$$

$$=\begin{pmatrix} \mathbf{u}_1 & \mathbf{u}_2 & . & . & . & \mathbf{u}_n \end{pmatrix}$$

where

$$\mathbf{u}_i=\begin{pmatrix} \langle b_1|a_i\rangle \\ \langle b_2|a_i\rangle \\ \langle b_3|a_i\rangle \\ . \\ . \\ \langle b_n|a_i\rangle \end{pmatrix} \qquad \text{(matrix form of eigenkets)}$$

Thus, we have

$$\boldsymbol{\alpha}=\mathbf{U}^{+}\boldsymbol{\beta}, \qquad \boldsymbol{\beta}=\mathbf{U}\boldsymbol{\alpha} \qquad \text{(matrix form)}$$

where

$$\mathbf{U} = \left(\mathbf{u}_1 \ \mathbf{u}_2 ......\mathbf{u}_n \ \right)$$

and

$$\mathbf{U}^+ = \begin{pmatrix} \mathbf{u}_1^* \\ \mathbf{u}_2^* \\ . \\ . \\ . \\ \mathbf{u}_n^* \end{pmatrix}$$

Note that

$$\boldsymbol{\beta}^+ \mathbf{A} \boldsymbol{\beta} = (\boldsymbol{\alpha}^+ \hat{\mathbf{U}}^+ \mathbf{A} \mathbf{U} \boldsymbol{\alpha}) = (\boldsymbol{\alpha}^+ \tilde{\mathbf{A}} \boldsymbol{\alpha})$$

where

$$\hat{\mathbf{U}}^+ \mathbf{A} \mathbf{U} = \begin{pmatrix} a_1 & 0 & . & . & . & 0 \\ 0 & a_2 & . & . & . & 0 \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & 0 & . & . & . & a_n \end{pmatrix} \qquad \text{(diagonal matrix)}$$

6.4 Example-1 (3x3 matrix)

Here we discuss a typical example, $\boldsymbol{A}$ is 3x3 matrix.

$$
\begin{aligned}
f &= 2(\beta_1^2 + \beta_2^2 + \beta_3^2 - \beta_1\beta_2 - \beta_2\beta_3 - \beta_3\beta_1) \\
&= \boldsymbol{\beta}^{+}\mathbf{A}\boldsymbol{\beta} \\
&= \begin{pmatrix} \beta_1^* & \beta_2^* & \beta_3^* \end{pmatrix} \mathbf{A} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} \\
&= \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 \end{pmatrix} \mathbf{A} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}
\end{aligned}
$$

Where β_1, β_2, and β_3 are real,

$$
\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}, \qquad \boldsymbol{\beta}^{+} = \begin{pmatrix} \beta_1^* & \beta_2^* & \beta_3^* \end{pmatrix} = \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 \end{pmatrix} = \boldsymbol{\beta}^{T},
$$

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

Eigenvalue problem of matrix $\boldsymbol{A}$ (we solve the problem using **Mathematica. The system is degenerate**)

$$
\mathbf{A}\phi_1 = a_1\phi_1, \qquad \mathbf{A}\phi_2 = a_2\phi_2, \qquad \mathbf{A}\phi_3 = a_3\phi_3.
$$

where the eigenvalues and eigenkets are as follows,

$$
a_1 = 3, \qquad \phi_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},
$$

$$a_2 = 3, \qquad \phi_2 = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix},$$

$$a_3 = 0, \qquad \phi_3 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

under the basis $\{|b_i\rangle\}$. The unitary matrix can be obtained as

$$\mathbf{U} = \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix}, \qquad \mathbf{U}^{+} = \begin{pmatrix} \phi_1^{+} \\ \phi_2^{+} \\ \phi_3^{+} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix}$$

$$\mathbf{U}^{+}\mathbf{U} = 1, \qquad \mathbf{U}^{+}\mathbf{A}\mathbf{U} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix} = \mathbf{U}\boldsymbol{\alpha} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix}\begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}\alpha_1 + \frac{1}{\sqrt{6}}\alpha_2 + \frac{1}{\sqrt{3}}\alpha_3 \\ -\frac{2}{\sqrt{6}}\alpha_2 + \frac{1}{\sqrt{3}}\alpha_3 \\ -\frac{1}{\sqrt{2}}\alpha_1 + \frac{1}{\sqrt{6}}\alpha_2 + \frac{1}{\sqrt{3}}\alpha_3 \end{pmatrix}$$

Thus, we have

$$
\begin{aligned}
f &= \boldsymbol{\beta}^{+}\mathbf{A}\boldsymbol{\beta} \\
&= \boldsymbol{\alpha}^{+}(\mathbf{U}^{+}\mathbf{A}\mathbf{U})\boldsymbol{\alpha} \\
&= \begin{pmatrix} \alpha_1^{*} & \alpha_2^{*} & \alpha_3^{*} \end{pmatrix} \begin{pmatrix} a_1 & 0 & 0 \\ 0 & a_2 & 0 \\ 0 & 0 & a_3 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} \\
&= a_1 |\alpha_1|^2 + a_2 |\alpha_2|^2 + a_3 |\alpha_3|^2 \\
&= 3\alpha_1^{\ 2} + 3\alpha_2^{\ 2} + 0\alpha_3^{\ 2}
\end{aligned}
$$

6.5 Example-2 4x4 matrix

We also discuu the second example; ***A*** is 4x4 matrix.

$$
\begin{aligned}
f &= \beta_1^{\ 2} + 2\beta_2^{\ 2} + 2\beta_3^{\ 2} + \beta_4^{\ 2} - 2\beta_1\beta_2 - 2\beta_2\beta_3 - 2\beta_3\beta_1 \\
&= \boldsymbol{\beta}^{+}\mathbf{A}\boldsymbol{\beta} \\
&= \begin{pmatrix} \beta_1^{*} & \beta_2^{*} & \beta_3^{*} & \beta_4^{*} \end{pmatrix} \mathbf{A} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix} \\
&= \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 & \beta_4 \end{pmatrix} \mathbf{A} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix}
\end{aligned}
$$

Where β_1, β_2, β_3 and β_4 are real,

$$
\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix} \qquad \boldsymbol{\beta}^{+} = \begin{pmatrix} \beta_1^{*} & \beta_2^{*} & \beta_3^{*} & \beta_4^{*} \end{pmatrix} = \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 & \beta_4 \end{pmatrix} = \boldsymbol{\beta}^{T}
$$

$$\mathbf{A}=\begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}.$$

Eigenvalue problem of matrix **A** (using **Mathematica**)

$$\mathbf{A}\phi_1 = a_1\phi_1, \qquad \mathbf{A}\phi_2 = a_2\phi_2,$$

$$\mathbf{A}\phi_3 = a_3\phi_3, \qquad \mathbf{A}\phi_4 = a_4\phi_4$$

The eigenvalues and eigenkets are obtained as follows,

$$a_1 = 2+\sqrt{2}, \qquad \phi_1 = \begin{pmatrix} \dfrac{1}{2\sqrt{2+\sqrt{2}}} \\ -\dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} \\ \dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} \\ -\dfrac{1}{2\sqrt{2+\sqrt{2}}} \end{pmatrix},$$

$$a_2 = 2, \qquad \phi_2 = \begin{pmatrix} \dfrac{1}{2} \\ -\dfrac{1}{2} \\ -\dfrac{1}{2} \\ \dfrac{1}{2} \end{pmatrix},$$

$$a_3 = 2-\sqrt{2}\,, \qquad \phi_3 = \begin{pmatrix} \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} \\ \frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} \\ -\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} \\ -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} \end{pmatrix}.$$

$$a_4 = 0\,, \qquad \phi_4 = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}.$$

The unitary matrix:

$$\mathbf{U} = \begin{pmatrix} \phi_1 & \phi_2 & \phi_3 & \phi_4 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2\sqrt{2+\sqrt{2}}} & \frac{1}{2} & \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & -\frac{1}{2} & \frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & -\frac{1}{2} & -\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}} & \frac{1}{2} \\ -\frac{1}{2\sqrt{2+\sqrt{2}}} & \frac{1}{2} & -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}} & \frac{1}{2} \end{pmatrix},$$

$$
\mathbf{U}^{+} = \begin{pmatrix} \phi_1^{+} \\ \phi_2^{+} \\ \phi_3^{+} \\ \phi_4^{+} \end{pmatrix}
= \begin{pmatrix}
\dfrac{1}{2\sqrt{2+\sqrt{2}}} & -\dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} & \dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} & -\dfrac{1}{2\sqrt{2+\sqrt{2}}} \\
\dfrac{1}{2} & -\dfrac{1}{2} & -\dfrac{1}{2} & \dfrac{1}{2} \\
\dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} & \dfrac{1}{2}\sqrt{1-\dfrac{1}{\sqrt{2}}} & -\dfrac{1}{2}\sqrt{1-\dfrac{1}{\sqrt{2}}} & -\dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} \\
\dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2} & \dfrac{1}{2}
\end{pmatrix}
$$

$$
\mathbf{U}^{+}\mathbf{U} = 1, \qquad \mathbf{U}^{+}\mathbf{A}\mathbf{U} = \begin{pmatrix}
2+\sqrt{2} & 0 & 0 & 0 \\
0 & 2 & 0 & 0 \\
0 & 0 & 2-\sqrt{2} & 0 \\
0 & 0 & 0 & 0
\end{pmatrix},
$$

$$
\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix} = \mathbf{U}\boldsymbol{\alpha} = \begin{pmatrix}
\dfrac{1}{2\sqrt{2+\sqrt{2}}} & \dfrac{1}{2} & \dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} & \dfrac{1}{2} \\
-\dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} & -\dfrac{1}{2} & \dfrac{1}{2}\sqrt{1-\dfrac{1}{\sqrt{2}}} & \dfrac{1}{2} \\
\dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} & -\dfrac{1}{2} & -\dfrac{1}{2}\sqrt{1-\dfrac{1}{\sqrt{2}}} & \dfrac{1}{2} \\
-\dfrac{1}{2\sqrt{2+\sqrt{2}}} & \dfrac{1}{2} & -\dfrac{1}{2}\sqrt{1+\dfrac{1}{\sqrt{2}}} & \dfrac{1}{2}
\end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{pmatrix},
$$

or

$$\begin{pmatrix}\beta_1\\\beta_2\\\beta_3\\\beta_4\end{pmatrix}=\begin{pmatrix}\frac{1}{2\sqrt{2+\sqrt{2}}}\alpha_1+\frac{1}{2}\alpha_2+\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}}\alpha_3+\frac{1}{2}\alpha_4\\ -\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}}\alpha_1-\frac{1}{2}\alpha_2+\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}}\alpha_3+\frac{1}{2}\alpha_4\\ \frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}}\alpha_1-\frac{1}{2}\alpha_2-\frac{1}{2}\sqrt{1-\frac{1}{\sqrt{2}}}\alpha_3+\frac{1}{2}\alpha_4\\ -\frac{1}{2\sqrt{2+\sqrt{2}}}\alpha_1+\frac{1}{2}\alpha_2-\frac{1}{2}\sqrt{1+\frac{1}{\sqrt{2}}}\alpha_3+\frac{1}{2}\alpha_4\end{pmatrix}.$$

Thus, we have

$$\begin{aligned}f&=\mathbf{\beta}^+\mathbf{A}\mathbf{\beta}\\&=\mathbf{\alpha}^+(\mathbf{U}^+\mathbf{A}\mathbf{U})\mathbf{\alpha}\\&=\begin{pmatrix}\alpha_1^* & \alpha_2^* & \alpha_3^* & \alpha_4^*\end{pmatrix}\begin{pmatrix}2+\sqrt{2} & 0 & 0 & 0\\0 & 2 & 0 & 0\\0 & 0 & 2-\sqrt{2} & 0\\0 & 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\alpha_1\\\alpha_2\\\alpha_3\\\alpha_4\end{pmatrix}\\&=a_1|\alpha_1|^2+a_2|\alpha_2|^2+a_3|\alpha_3|^2+a_4|\alpha_4|^2\\&=(2+\sqrt{2})\alpha_1^{\ 2}+2\alpha_2^{\ 2}+(2-\sqrt{2})\alpha_3^{\ 2}+0\alpha_4^{\ 2}\end{aligned}$$

7. Equivalence with Schrödinger equation

The Schrödinger equation is given by

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle=\hat{H}\left|\psi(t)\right\rangle.$$

For an infinitesimal time interval ε, we can write

$$\left|\psi(\varepsilon)\right\rangle-\left|\psi(0)\right\rangle=-\frac{i\varepsilon}{\hbar}\hat{H}\left|\psi(0)\right\rangle,$$

from the definition of the derivative, or