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Pauli Spin Matrices

Carl W. David

University of Connecticut, Carl.David@uconn.edu

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The Pauli spin matrices are

\[ S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]

\[ S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \]

\[ S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

(2.1)

but we will work with their unitless equivalents

\[ \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]

\[ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \]

\[ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

(2.2)

where we will be using this matrix language to discuss a spin 1/2 particle.

We note the following construct:

\[ \sigma_x \sigma_y - \sigma_y \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]

which is

\[ \sigma_x \sigma_y - \sigma_y \sigma_x = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \]

which is, finally,

\[ \sigma_x \sigma_y - \sigma_y \sigma_x = \begin{pmatrix} 2i & 0 \\ 0 & 2i \end{pmatrix} = 2i \sigma_z \]

We can do the same again,

\[ \sigma_x \sigma_z - \sigma_z \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]

which is

\[ \sigma_x \sigma_z - \sigma_z \sigma_x = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \]

which is, finally,

\[ \sigma_x \sigma_z - \sigma_z \sigma_x = \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} = -2i \sigma_y \]

Summarizing, we have

\[ [\sigma_x, \sigma_y] = 2i \sigma_z \]

and, by cyclic permutation.

\[ [\sigma_y, \sigma_z] = 2i \sigma_x \]

\[ [\sigma_z, \sigma_x] = 2i \sigma_y \]

Next, we compute \( \sigma^2 \) i.e.,

\[ \sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = \]

\[ \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) + \left( \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right) \left( \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right) + \left( \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \left( \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \]

(2.3)

\[ \sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = \]

\[ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix} \]

(2.4)
We need the commutator of $\sigma^2$ with each component of $\sigma$. We obtain
\[
[\sigma^2, \sigma_x] = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} - \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix} = 0
\]
with the same results for $\sigma_y$ and $\sigma_z$, since $\sigma^2$ is diagonal. Since the three components of spin individually do not commute, i.e., $[\sigma_x, \sigma_y] \neq 0$ as an example, we know that the three components of spin can not simultaneously be measured. A choice must be made as to what we will simultaneously measure, and the traditional choice is $\sigma^2$ and $\sigma_z$. This is analogous to the $L^2$ and $L_z$ choice made in angular momentum.

Choosing $\sigma^2$ and $\sigma_z$ we have
\[
\sigma^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 3 \begin{pmatrix} 1 \\ 0 \end{pmatrix}
\]
(with a similar result for $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$)

and
\[
\sigma_z \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}
\]
again, with a similar (the eigenvalue is then -1) result for the other component.

This implies that a matrix representative of $\sigma^2$ would be (in this representation)
\[
\sigma^2 = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}
\]
and
\[
\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]
with the two eigenstates:
\[
\begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \alpha
\]
and
\[
\begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \beta
\]
corresponding to “spin up” and “spin down”, which is sometimes designated $\alpha$ and $\beta$.

We then have
\[
\sigma^2 \alpha = 3\alpha
\]
and
\[
\sigma^2 \beta = 3\beta
\]
while
\[
\sigma_z \alpha = 1\alpha
\]
and
\[
\sigma_z \beta = -1\beta
\]
We note in passing that
\[
\sigma_x \alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \beta
\]

III. LADDER OPERATORS IN 1-SPIN SYSTEMS

It is appropriate to form ladder operators, just as we did with angular momentum, i.e.,
\[
\sigma^+ = \sigma_x + i\sigma_y
\]
and
\[
\sigma^- = \sigma_x - i\sigma_y
\]
which in matrix form would be
\[
\sigma^+ = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + i \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}
\]
Clearly
\[
\sigma^+ \beta = 2\alpha
\]
and
\[
\sigma^+ \alpha = 0
\]
as expected. Similar results for the down ladder operator follow immediately.
\[
\sigma^- = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - i \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix}
\]
Clearly
\[
\sigma^- \alpha = 2\beta
\]
These are the analog of $L^+$ and $L^-$ operators in standard angular momentum discussions.

IV. ANTICOMMUTATIVITY

We need to observe a particularly strange behaviour of spin operators (and their matrix representatives).
\[
\sigma_x \sigma_y + \sigma_y \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} + \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]
which is
\[
\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} + \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \rightarrow 0
\]
This is known as “anti-commutation”, i.e., not only do the spin operators not commute amongst themselves, but the anticommutate! They are strange beasts.

V. 2 SPIN SYSTEMS

With 2 spin systems we enter a different world. Let’s make a table of possible values:
It makes sense to construct some kind of “4-dimensional” representation for this double spin system, i.e.,

\[
\begin{align*}
\alpha(1)\alpha(2) & \rightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \\
\beta(1)\beta(2) & \rightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}
\end{align*}
\]

These are the “unit vectors” in the space of interest. Each unit vector stands for a meaningful combination of the spins. It is sometimes shorter to drop the (1) and (2) and just agree that the left hand designator points to spin-1 and the right hand one to spin-2.

Summarizing, in all the relevant notations, we have

<table>
<thead>
<tr>
<th>spin_1</th>
<th>spin_2</th>
<th>denoted as</th>
<th>4-vector</th>
</tr>
</thead>
</table>
| 1/2    | 1/2    | \(\alpha(1)\alpha(2)\) | \[
\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}
\]
| 1/2    | -1/2   | \(\alpha(1)\beta(2)\) | \[
\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}
\]
| -1/2   | 1/2    | \(\beta(1)\alpha(2)\) | \[
\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}
\]
| -1/2   | -1/2   | \(\beta(1)\beta(2)\) | \[
\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\]

Now we need the matrix designators of the system’s spin, the overall spin. To do this, we adopt the so-called vector model for spin, i.e.,

\[
\vec{\Sigma} = \vec{\sigma}_1 + \vec{\sigma}_2
\]

What is the effect of \(\Sigma\) on the \(\alpha(1)\alpha(2)\) state? We have

\[
\Sigma_x \alpha(1)\alpha(2) = \Sigma_x \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}
\]
\[ \Sigma_x \alpha(1) \alpha(2) = (\sigma_x + \sigma_x) \alpha(1) \alpha(2) = \alpha(2) \sigma_x \alpha(1) + \alpha(1) \sigma_x \alpha(2) = \left\{ \alpha(2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}_1 + \left\{ \alpha(1) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}_2 \]
or
\[ \Sigma_x \alpha(1) \alpha(2) = (\sigma_x + \sigma_x) \alpha(1) \alpha(2) = \alpha(2) \sigma_x \alpha(1) + \alpha(1) \sigma_x \alpha(2) = \left\{ \alpha(2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}_1 + \left\{ \alpha(1) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\}_2 \]

which we might re-write as where each spin matrix operates solely on the appropriate spin function. (You may prefer to remember that \( \sigma_x \alpha \to \beta \), and vice versa).

We then have

\[ \Sigma_x \alpha(1) \alpha(2) = \alpha(2) \beta(1) + \alpha(1) \beta(2) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \]

which means that the 4x4 matrix representative of \( \Sigma_x \) must have as its first row and column:

\[
\begin{pmatrix}
0 & 1 & 1 & 0 \\
1 & ? & ? & ? \\
1 & ? & ? & ? \\
0 & ? & ? & ? \\
\end{pmatrix}
\]

\[ \Sigma_x \alpha \alpha = \left( \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & ? & ? & ? \\ 1 & ? & ? & ? \\ 0 & ? & ? & ? \end{pmatrix} \right) \otimes \left( \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \right) = \left( \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \right) + \left( \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right) \]

which would be

\[ < 2 | \Sigma_x | 1 >= \alpha(1) \beta(2) \otimes \Sigma_x \otimes (\alpha(1) \alpha(2)) \]

which is

\[ < 2 | \Sigma_x | 1 >= \alpha(1) \beta(2) \otimes (\beta(1) \alpha(2) + \alpha(1) \beta(2)) = 1 \]

Similarly we obtain

\[ \Sigma_y = \begin{pmatrix} 0 & -i & -1 & 0 \\
i & 0 & 0 & -i \\
i & 0 & 0 & -i \\
0 & i & i & 0 \end{pmatrix} \]
and, finally,

\[ \Sigma_z = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} \]

It is interesting to form \( \vec{\Sigma} \cdot \vec{\Sigma} \), i.e.,

\[ \Sigma^2 = \Sigma_z^2 + \Sigma_y^2 + \Sigma_2^2 = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}^2 + \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & -i \\ i & 0 & 0 & -i \\ 0 & i & i & 0 \end{pmatrix}^2 + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} \]

which is

\[ \Sigma^2 = \begin{pmatrix} 2 & 0 & 0 & 2 \\ 0 & 2 & 2 & 0 \\ 0 & 2 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{pmatrix} + \begin{pmatrix} 2 & 0 & 0 & -2 \\ 0 & 2 & 2 & 0 \\ 0 & 2 & 2 & 0 \\ 2 & 0 & 0 & 2 \end{pmatrix} + \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \]

and simultaneously, \( \alpha(1)\alpha(2) \) is an eigenfunction of \( \Sigma_z \):

\[ \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \]

This means that \( \alpha(1)\alpha(2) \) is an observable state of the system (as is \( \beta(1)\beta(2) \)). Notice further that neither \( \alpha(1)\beta(2) \) nor \( \beta(1)\alpha(2) \) is an eigenfunction of either \( \Sigma^2 \) or \( \Sigma_z \). Instead, linear combinations of these two states are appropriate, i.e.,

\[ \Sigma^2(\alpha(1)\beta(2) + \beta(1)\alpha(1)) = \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 4 & 4 & 0 \\ 0 & 4 & 4 & 0 \\ 0 & 0 & 0 & 8 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \]

where the bracketing has to be studied to see that we are adding the two column vectors before multiplying from the left with the spin operator. The result is

\[ \begin{pmatrix} 0 \\ 8 \\ 0 \\ 0 \end{pmatrix} = 8 \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \]
which shows that the functions $\alpha(1)\beta(2) + \alpha(2)\beta(1)$ are eigenfunctions of $\Sigma^2$ as expected.

The other linear combination, $\alpha(1)\beta(2) - \alpha(1)\beta(1)$ works in the same manner.

\[
\Sigma^2(\alpha(1)\beta(2) - \beta(1)\alpha(1)) = \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 4 & 4 & 0 \\ 0 & 4 & 4 & 0 \\ 0 & 0 & 0 & 8 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \text{zero} \otimes \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}
\]

and

\[
\Sigma_z(\alpha(1)\beta(2) - \beta(1)\alpha(2)) = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \text{zero} \times \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}
\]

This single state stands out from the other three, i.e., it is the singlet state, while the other three are components of the triplet state. The singlet state corresponds to an overall spin of zero, while the triplet state corresponds to an overall spin of 1.

VI. DIAGONALIZING THE $\Sigma^2$ MATRIX

Consider the Equation

\[
\begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 4 & 4 & 0 \\ 0 & 4 & 4 & 0 \\ 0 & 0 & 0 & 8 \end{pmatrix} \otimes \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \gamma \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}
\]

Where we seek the set $\{c_i\}$, the eigenvectors of this operator (and we seek the associated eigenvalues $\gamma$).

Traditionally, we re-write this equation as

\[
\begin{pmatrix} 8 - \gamma & 0 & 0 & 0 \\ 0 & 4 - \gamma & 4 & 0 \\ 0 & 4 & 4 - \gamma & 0 \\ 0 & 0 & 0 & 8 - \gamma \end{pmatrix} \otimes \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = 0
\]

and use Cramer’s rule to argue that the determinant associated with this matrix must be zero so that the solutions are unique. We then have

\[
\begin{vmatrix} 8 - \gamma & 0 & 0 & 0 \\ 0 & 4 - \gamma & 4 & 0 \\ 0 & 4 & 4 - \gamma & 0 \\ 0 & 0 & 0 & 8 - \gamma \end{vmatrix} = 0
\]

which expands into the quartic equation

\[
(8 - \gamma) \begin{vmatrix} 4 - \gamma & 4 & 0 \\ 4 & 4 - \gamma & 0 \\ 0 & 0 & 8 - \gamma \end{vmatrix} = 0
\]

or

\[
(8 - \gamma)^2 \begin{vmatrix} 4 - \gamma & 4 \\ 4 & 4 - \gamma \end{vmatrix} = 0
\]

which is, finally,

\[
\sqrt{(4 - \gamma)^2} = \pm 4
\]

which yields two more roots, one $\gamma = 8$ and the other $\gamma = 0$. As if we didn’t know that!

The linear combinations, $\alpha(1)\beta(2) \pm \beta(1)\alpha(2)$ come out of this argument!

VII. SIMILARITY TRANSFORMATION ILLUSTRATED

The eigenvectors for this problem are

\[
\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\]

in normalized form. Juxtaposing these four eigenvectors we obtain a matrix, $T$, of the form

\[
T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 1 \end{pmatrix}
\]
and, “spinning” (pun, pun, pun) around the main diagonal, we have

\[
T^\dagger = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\
0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

...(the adjoint) such that the construct \(T^\dagger S^2_{op} T\) is

\[
T^\dagger S^2_{op} T = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\
0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} \otimes \begin{pmatrix}
8 & 0 & 0 & 0 \\
0 & 4 & 4 & 0 \\
0 & 4 & 4 & 0 \\
0 & 0 & 0 & 8
\end{pmatrix} \otimes \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

which is

\[
T^\dagger S^2_{op} T = \begin{pmatrix}
8 & 0 & 0 & 0 \\
0 & 8 & 0 & 0 \\
0 & 0 & 8 & 0 \\
0 & 0 & 0 & 8
\end{pmatrix}
\]

The conjoined eigenvectors constructed to make the matrix \(T\), create a matrix which, when operating on the \(S^2_{op}\) matrix representative of \(S^2\) in the manner indicated, diagonalizes it. The composite operation is known as a similarity transformation.