Section 2. Enter Tmat.

The matrix Tmat defined next is the TET example from Section 15.3 of TapeTape2021. It is also Eq (76) of TapeTape2022.
Change Tmat to suit yourself, but of course Tmat must be symmetric. Tmat is the matrix $[T]_{\mathbb{B}\mathbb{B}}$ of your elastic map T with respect to the basis $\mathbb{B}$.

In[1312]:=

```
Print[DateSequence[DateList[], "yes"]];
```

$$\text{Tmat} = \frac{1}{64}\begin{pmatrix} 168 & 4\sqrt{6} & -40 & 6\sqrt{6} & 6\sqrt{2} & 0 \\ 4\sqrt{6} & 324 & -4\sqrt{6} & -42 & -14\sqrt{3} & 16\sqrt{3} \\ -40 & -4\sqrt{6} & 168 & -6\sqrt{6} & -6\sqrt{2} & 0 \\ 6\sqrt{6} & -42 & -6\sqrt{6} & 233 & 35\sqrt{3} & -8\sqrt{3} \\ 6\sqrt{2} & -14\sqrt{3} & -6\sqrt{2} & 35\sqrt{3} & 163 & -8 \\ 0 & 16\sqrt{3} & 0 & -8\sqrt{3} & -8 & 352 \end{pmatrix};$$

```
denominator = 64;
(* Tmat=TmatBrown; denominator=1; *)
```

3-19-2024 20:36

Section 3. Output.

Choose one :

In[1314]:=

```
WantDetails = "NoWantDetails"
```

Out[1314]=

NoWantDetails

In[1315]:=

```
WantDetails = "WantDetails"
```

Out[1315]=

WantDetails

Σ = MONO

In[1316]:=

```
OutputFor[Tmat, MONO]
```

3-19-2024 20:36

NMinimize = $\{6.94931\times10^{-9}, \{\theta\to 0., \sigma\to 2.00611, \phi\to 0.785398\}\}$

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{MONO}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are $\{0., 0., 45.\}$)

$$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} 0.707107 & 0 & 0.707107 \\ 0 & 1. & 0 \\ -0.707107 & 0 & 0.707107 \end{pmatrix}$$ (A MONO

-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{MONO}(U))$)

$\beta^{T}_{MONO} = 0$ (Angle between T and $\mathcal{T}_{MONO}$. The initial $\beta^{T}_{MONO} = 7.2\times10^{-10}$ is here chopped to zero, since the chop threshold is set at 0.01°)

Since $\beta^{T}_{MONO} = 0$, T is assigned symmetry at least MONO.

$\mathcal{V}_{MONO}(U_0)$ contains T

$d(T, \mathcal{T}_{MONO}) = 6.9\times10^{-9}$ (Distance from T to $\mathcal{T}_{MONO}$)

$$T_{MONO} = [\overline{U_0}]^T[T][\overline{U_0}] = \begin{pmatrix} 2. & 0 & 0 & 0 & 0 & 0 \\ 0 & 2. & 0 & 0 & 0 & 0 \\ 0 & 0 & 3.25 & -0.433013 & 0 & 0 \\ 0 & 0 & -0.433013 & 3.75 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.5 & -0.5 \\ 0 & 0 & 0 & 0 & -0.5 & 5.5 \end{pmatrix}$$

(Should be a MONO-ref matrix for T. If not, consider decreasing ChopT.)

Σ = ORTH

In[1317]:=

```
OutputFor[Tmat, ORTH]
```

3-19-2024 20:36

NMinimize = $\{4.98692\times10^{-8}, \{\theta\to1.1832, \sigma\to-0.857072, \phi\to1.93216\}\}$

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{ORTH}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are $\{67.8, -49.1, 110.7\}$)

$$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} 0.612372 & -0.707107 & 0.353553 \\ -0.5 & 0 & 0.866025 \\ -0.612372 & -0.707107 & -0.353553 \end{pmatrix}$$ (A ORTH

-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{ORTH}(U))$)

$\beta^T_{ORTH} = 0$ (Angle between T and $\mathcal{T}_{ORTH}$. The initial $\beta^T_{ORTH} = 5.1\times10^{-9}$ is here chopped to zero, since the chop threshold is set at 0.01°)

Since $\beta^T_{ORTH} = 0$, T is assigned symmetry at least ORTH.

$\mathcal{V}_{ORTH}(U_0)$ contains T

$d(T, \mathcal{T}_{ORTH}) = 4.99\times10^{-8}$ (Distance from T to $\mathcal{T}_{ORTH}$)

$$T_{ORTH} = [\overline{U_0}]^T[T][\overline{U_0}] = \begin{pmatrix} 2. & 0 & 0 & 0 & 0 & 0 \\ 0 & 4. & 0 & 0 & 0 & 0 \\ 0 & 0 & 2. & 0 & 0 & 0 \\ 0 & 0 & 0 & 4.875 & 1.08253 & 0.433013 \\ 0 & 0 & 0 & 1.08253 & 3.625 & 0.25 \\ 0 & 0 & 0 & 0.433013 & 0.25 & 5.5 \end{pmatrix}$$

(Should be a ORTH-ref matrix for T. If not, consider decreasing ChopT.)

Σ = TET

In[1318]:=

```
OutputFor[Tmat, TET]
```

3-19-2024 20:37

NMinimize = $\{8.82384\times10^{-8}, \{\theta\to3.14159, \sigma\to2.87979, \phi\to2.35619\}\}$

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{TET}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are $\{180., 165., 135.\}$)

$$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} -0.683013 & -0.183013 & -0.707107 \\ -0.258819 & 0.965926 & 0 \\ 0.683013 & 0.183013 & -0.707107 \end{pmatrix}$$ (A TET

-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{TET}(U))$)

$\beta^{T}_{TET} = 0$ (Angle between T and $\mathcal{T}_{TET}$. The initial $\beta^{T}_{TET} = 9.1\times10^{-9}$ is here chopped to zero, since the chop threshold is set at 0.01°)

Since $\beta^{T}_{TET} = 0$, T is assigned symmetry at least TET.

$\mathcal{V}_{TET}(U_0)$ contains T

$d(T, \mathcal{T}_{TET}) = 8.8\times10^{-8}$ (Distance from T to $\mathcal{T}_{TET}$)

$$T_{TET} = [\overline{U_0}]^T[T][\overline{U_0}] = \begin{pmatrix} 2. & 0 & 0 & 0 & 0 & 0 \\ 0 & 2. & 0 & 0 & 0 & 0 \\ 0 & 0 & 3. & 0 & 0 & 0 \\ 0 & 0 & 0 & 4. & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.5 & -0.5 \\ 0 & 0 & 0 & 0 & -0.5 & 5.5 \end{pmatrix}$$ (Should be a

TET-ref matrix for T. If not, consider decreasing ChopT.)

Σ = CUBE

In[1319]:=

```
OutputFor[Tmat, CUBE]
```

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NMinimize = $\{1.51383, \{\theta \to 1.75805, \sigma \to -0.802729, \phi \to 1.38675\}\}$

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{CUBE}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are $\{100.7, -46., 79.5\}$)

$$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} 0.683013 & -0.707107 & -0.183013 \\ 0.258819 & 0 & 0.965926 \\ -0.683013 & -0.707107 & 0.183013 \end{pmatrix}$$ (A CUBE

-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{CUBE}(U))$)

$\beta^{T}_{CUBE} = 0.157 = 8.98^\circ$ (Angle between T and $\mathcal{T}_{CUBE}$)

$\mathcal{V}_{CUBE}(U_0)$ contains a closest map to T in $\mathcal{T}_{CUBE}$

$d(T, \mathcal{T}_{CUBE}) = 1.514$ (Distance from T to $\mathcal{T}_{CUBE}$)

Crude min check: Five smallest β values for 10 000 random rotations are $\{9.15639, 9.23062, 9.35297, 9.46136, 9.48536\}$

If $9.15639 \geq \beta^{T}_{CUBE} = 8.98287$, then probably OK. Otherwise minimization has failed.

$$P(T, \mathcal{V}_{CUBE}(U_0)) = \begin{pmatrix} 2.63542 & 0.369975 & -0.302083 & 0.554963 & 0.320408 & 0 \\ 0.369975 & 4.59896 & -0.369975 & -0.226562 & -0.130806 & 0 \\ -0.302083 & -0.369975 & 2.63542 & -0.554963 & -0.320408 & 0 \\ 0.554963 & -0.226562 & -0.554963 & 3.80599 & 0.850238 & 0 \\ 0.320408 & -0.130806 & -0.320408 & 0.850238 & 2.82422 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5.5 \end{pmatrix}$$

(a closest elastic map to T having symmetry at least CUBE)

Σ = TRIG

In[1320]:=

```
OutputFor[Tmat, TRIG]
```

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NMinimize = $\{0.707107, \{\theta \to 3.14159, \sigma \to -2.69718, \phi \to 2.35619\}\}$

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{TRIG}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are $\{180., -154.5, 135.\}$)

$$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} -0.638421 & 0.304004 & -0.707107 \\ 0.429927 & 0.902864 & 0 \\ 0.638421 & -0.304004 & -0.707107 \end{pmatrix}$$ (A TRIG

-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{TRIG}(U))$)

$\beta^{T}_{TRIG} = 0.073 = 4.18^{\circ}$ (Angle between T and $\mathcal{T}_{TRIG}$)

$\mathcal{V}_{TRIG}(U_0)$ contains a closest map to T in $\mathcal{T}_{TRIG}$

$d(T, \mathcal{T}_{TRIG}) = 0.707$ (Distance from T to $\mathcal{T}_{TRIG}$)

Crude min check: Five smallest β values for 10 000 random rotations are $\{4.21099, 4.43525, 4.45716, 4.51229, 4.56295\}$

If $4.21099 \geq \beta^{T}_{TRIG} = 4.18244$, then probably OK. Otherwise minimization has failed.

$$P(T, \mathcal{V}_{TRIG}(U_0)) = \begin{pmatrix} 2.75 & 0 & -0.75 & 0 & 0 & 0 \\ 0 & 5. & 0 & -0.75 & -0.433013 & 0.433013 \\ -0.75 & 0 & 2.75 & 0 & 0 & 0 \\ 0 & -0.75 & 0 & 3.5 & 0.866025 & -0.216506 \\ 0 & -0.433013 & 0 & 0.866025 & 2.5 & -0.125 \\ 0 & 0.433013 & 0 & -0.216506 & -0.125 & 5.5 \end{pmatrix}$$

(a closest elastic map to T having symmetry at least TRIG)

Σ = XISO

In[1321]:=

```
OutputFor[Tmat, XISO]
```

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NMinimize = {0.707107, {$\theta \to 3.14159$, $\sigma \to -2.36917$, $\phi \to 2.35619$}}

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{XISO}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are {180., 0., 135.})

$$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} 0.707107 & 0 & -0.707107 \\ 0 & -1. & 0 \\ -0.707107 & 0 & -0.707107 \end{pmatrix}$$ (A XISO

-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{XISO}(U))$)

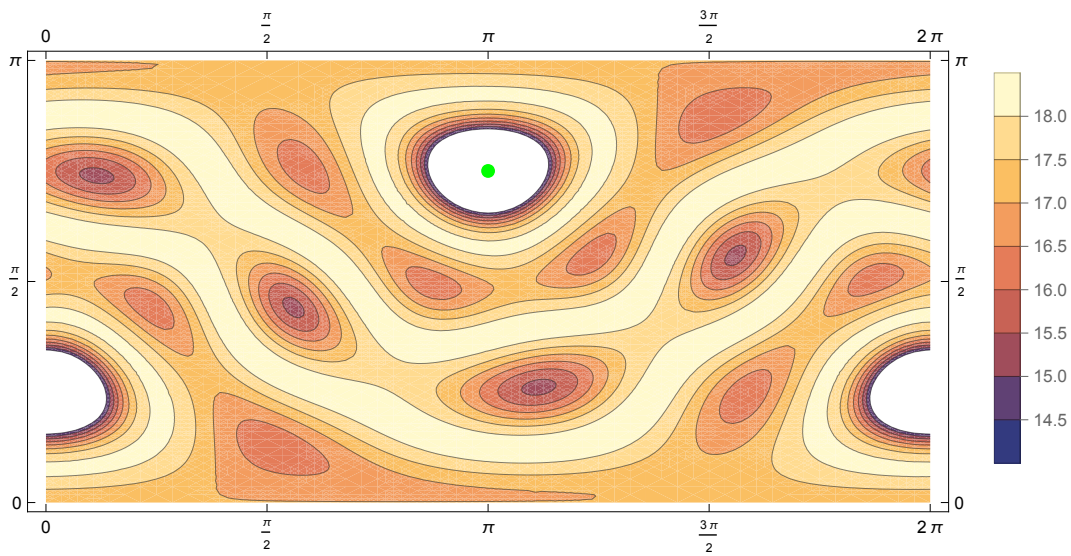
$\beta^{T}_{XISO} = 0.073 = 4.18^{\circ}$ (Angle between T and $\mathcal{T}_{XISO}$)

$\mathcal{V}_{XISO}(U_0)$ contains a closest map to T in $\mathcal{T}_{XISO}$

$d(T, \mathcal{T}_{XISO}) = 0.707$ (Distance from T to $\mathcal{T}_{XISO}$)

Does the green point look like a correct
GLOBAL minimum? If not, the minimization has failed.

Uniqueness (or not) of the closest XISO map is usually obvious from the contour plot.



$$P(T, \mathcal{V}_{XISO}(U_0)) = \begin{pmatrix} 2.75 & 0 & -0.75 & 0 & 0 & 0 \\ 0 & 5. & 0 & -0.75 & -0.433013 & 0.433013 \\ -0.75 & 0 & 2.75 & 0 & 0 & 0 \\ 0 & -0.75 & 0 & 3.5 & 0.866025 & -0.216506 \\ 0 & -0.433013 & 0 & 0.866025 & 2.5 & -0.125 \\ 0 & 0.433013 & 0 & -0.216506 & -0.125 & 5.5 \end{pmatrix}$$

(a closest elastic map to T having symmetry at least XISO)

Σ = ISO

In[1322]:=

```
OutputFor[Tmat, ISO]
```

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$\mathcal{V}_{\mathrm{ISO}}(\mathrm{U}) = \mathcal{V}_{\mathrm{ISO}}(\mathrm{I})$, independent of U, so the function U $\longrightarrow$ $\mathrm{d}(\mathrm{T}, \mathcal{V}_{\mathrm{ISO}}(\mathrm{U})) = \mathrm{d}(\mathrm{T}, \mathcal{T}_{\mathrm{ISO}})$ is constant.

$\mathrm{d}(\mathrm{T}, \mathcal{T}_{\mathrm{ISO}}) = \sqrt{\frac{93}{10}}$ (Distance from T to $\mathcal{T}_{\mathrm{ISO}}$)

$\beta_{\mathrm{ISO}}^{\square\,\mathrm{T}} = 0.32 = 18.33^{\circ}$ (Angle between T and $\mathcal{T}_{\mathrm{ISO}}$)

$$\mathrm{P}(\mathrm{T},\mathcal{V}_{\mathrm{ISO}}(\mathrm{I})) = \begin{pmatrix} 3.3 & 0. & 0. & 0. & 0. & 0. \\ 0. & 3.3 & 0. & 0. & 0. & 0. \\ 0. & 0. & 3.3 & 0. & 0. & 0. \\ 0. & 0. & 0. & 3.3 & 0. & 0. \\ 0. & 0. & 0. & 0. & 3.3 & 0. \\ 0. & 0. & 0. & 0. & 0. & 5.5 \end{pmatrix}$$

(The closest elastic map to T having symmetry ISO)

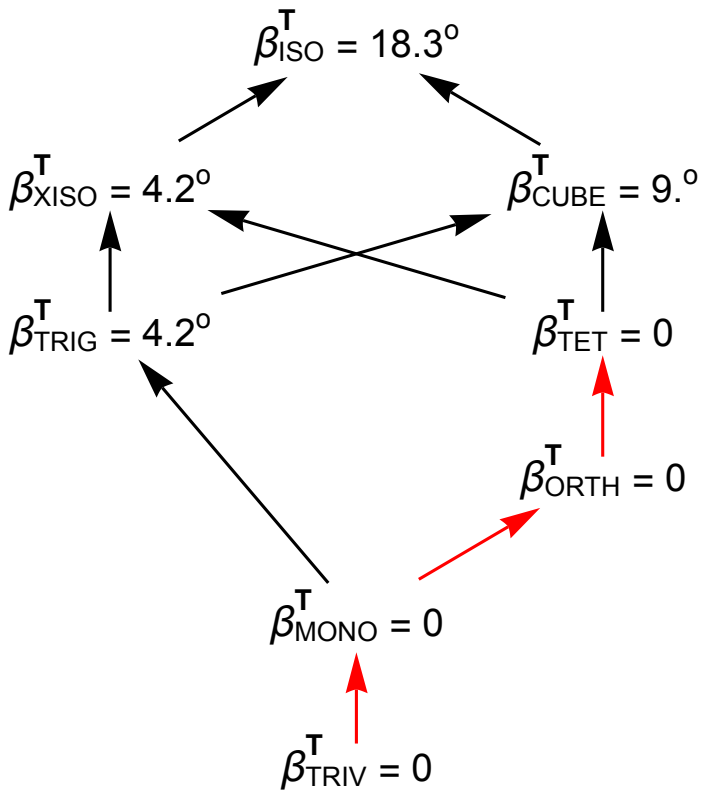
Lamé parameters for $\mathrm{P}(\mathrm{T},\mathcal{V}_{\mathrm{ISO}}(\mathrm{I}))$ are $\lambda = \frac{11}{15}$ and $\mu = \frac{33}{20}$, bulk modulus $\kappa = \frac{11}{6}$, Poisson ratio $= \frac{2}{13}$

If $\beta_{\Sigma}^{T} = 999$ in the lattice, then you failed to evaluate OutputFor[Tmat, Σ] above.

In[1323]:=

```
LatticeOfDTs[Tmat]
Print["[T] = ", 1/denominator, MatrixForm[denominator Tmat]]
ChopT = 0.01°
```

Out[1323]=



$$[T] = \frac{1}{64}\begin{pmatrix} 168 & 4\sqrt{6} & -40 & 6\sqrt{6} & 6\sqrt{2} & 0 \\ 4\sqrt{6} & 324 & -4\sqrt{6} & -42 & -14\sqrt{3} & 16\sqrt{3} \\ -40 & -4\sqrt{6} & 168 & -6\sqrt{6} & -6\sqrt{2} & 0 \\ 6\sqrt{6} & -42 & -6\sqrt{6} & 233 & 35\sqrt{3} & -8\sqrt{3} \\ 6\sqrt{2} & -14\sqrt{3} & -6\sqrt{2} & 35\sqrt{3} & 163 & -8 \\ 0 & 16\sqrt{3} & 0 & -8\sqrt{3} & -8 & 352 \end{pmatrix}$$

From the lattice and the appropriate *U* you get the symmetry group of T. See Theorem 3 of TapeTape2022.

In[1325]:=

```
FromTheorem3[Tmat]
```

The symmetry classes Σ with $\beta_{\Sigma}^{T} = 0$ are {TRIV, MONO, ORTH, TET}

The symmetry class for T is TET

The symmetry group for T is $U\,\mathbb{U}_{TET}\,U^{T}$

, where U = UT[Tmat,TET] = $\begin{pmatrix} -0.683013 & -0.183013 & -0.707107 \\ -0.258819 & 0.965926 & 0 \\ 0.683013 & 0.183013 & -0.707107 \end{pmatrix}$

As an example, ZRot[π/2] is in $\mathbb{U}_{TET}$, so $V = U$ ZRot[π/2]

U^T should be *a* symmetry of T.

In[1326]:=

```
V = UT[Tmat, TET].ZRot[π / 2].Transpose[UT[Tmat, TET]];
MatrixForm[Chop[V]]
MatrixForm[Chop[MatrixUbar[V].Tmat.Transpose[MatrixUbar[V]] - Tmat, 10^-7]]
```

Out[1327]//MatrixForm=

$$\begin{pmatrix} 0.5 & 0.707107 & 0.5 \\ -0.707107 & 0 & 0.707107 \\ 0.5 & -0.707107 & 0.5 \end{pmatrix}$$

Out[1328]//MatrixForm=

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

Addendum 1a: output from OutputFor[Tmat, MONO] This shows some of the quantities and capabilities that are available after running OutputFor.

In[1329]:=

```
WantDetails = "WantDetails"
```

Out[1329]=

WantDetails

In[1330]:=

```
Σ = MONO;
```

In[1331]:=

```
Print["Tmat = ", MatrixForm[Tmat], " = ", MatrixForm[N[Tmat]]];
```

$$\text{Tmat} = \begin{pmatrix} \frac{21}{8} & \frac{\sqrt{\frac{3}{2}}}{8} & -\frac{5}{8} & \frac{3\sqrt{\frac{3}{2}}}{16} & \frac{3}{16\sqrt{2}} & 0 \\ \frac{\sqrt{\frac{3}{2}}}{8} & \frac{81}{16} & -\frac{\sqrt{\frac{3}{2}}}{8} & -\frac{21}{32} & -\frac{7\sqrt{3}}{32} & \frac{\sqrt{3}}{4} \\ -\frac{5}{8} & -\frac{\sqrt{\frac{3}{2}}}{8} & \frac{21}{8} & -\frac{3\sqrt{\frac{3}{2}}}{16} & -\frac{3}{16\sqrt{2}} & 0 \\ \frac{3\sqrt{\frac{3}{2}}}{16} & -\frac{21}{32} & -\frac{3\sqrt{\frac{3}{2}}}{16} & \frac{233}{64} & \frac{35\sqrt{3}}{64} & -\frac{\sqrt{3}}{8} \\ \frac{3}{16\sqrt{2}} & -\frac{7\sqrt{3}}{32} & -\frac{3}{16\sqrt{2}} & \frac{35\sqrt{3}}{64} & \frac{163}{64} & -\frac{1}{8} \\ 0 & \frac{\sqrt{3}}{4} & 0 & -\frac{\sqrt{3}}{8} & -\frac{1}{8} & \frac{11}{2} \end{pmatrix} =$$

$$\begin{pmatrix} 2.625 & 0.153093 & -0.625 & 0.22964 & 0.132583 & 0. \\ 0.153093 & 5.0625 & -0.153093 & -0.65625 & -0.378886 & 0.433013 \\ -0.625 & -0.153093 & 2.625 & -0.22964 & -0.132583 & 0. \\ 0.22964 & -0.65625 & -0.22964 & 3.64063 & 0.947215 & -0.216506 \\ 0.132583 & -0.378886 & -0.132583 & 0.947215 & 2.54688 & -0.125 \\ 0. & 0.433013 & 0. & -0.216506 & -0.125 & 5.5 \end{pmatrix}$$

In[1332]:=

```
OutputFor[Tmat, Σ]
```

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NMinimize = $\{6.94931\times10^{-9}, \{\theta\to 0., \sigma\to 2.00611, \phi\to 0.785398\}\}$

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{\text{MONO}}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are $\{0., 0., 45.\}$)

$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} 0.707107 & 0 & 0.707107 \\ 0 & 1. & 0 \\ -0.707107 & 0 & 0.707107 \end{pmatrix}$ (A MONO-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{\text{MONO}}(U))$)

$\beta^{T}_{\text{MONO}} = 0$ (Angle between T and $\mathcal{T}_{\text{MONO}}$. The initial $\beta^{T}_{\text{MONO}} = 7.2\times10^{-10}$ is here chopped to zero, since the chop threshold is set at 0.01°)

Since $\beta^{T}_{\text{MONO}} = 0$, T is assigned symmetry at least MONO.

$\mathcal{V}_{\text{MONO}}(U_0)$ contains T

$d(T, \mathcal{T}_{\text{MONO}}) = 6.9\times10^{-9}$ (Distance from T to $\mathcal{T}_{\text{MONO}}$)

$$T_{\text{MONO}} = [\overline{U_0}]^T[T][\overline{U_0}] = \begin{pmatrix} 2. & 0 & 0 & 0 & 0 & 0 \\ 0 & 2. & 0 & 0 & 0 & 0 \\ 0 & 0 & 3.25 & -0.433013 & 0 & 0 \\ 0 & 0 & -0.433013 & 3.75 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.5 & -0.5 \\ 0 & 0 & 0 & 0 & -0.5 & 5.5 \end{pmatrix}$$

(Should be a MONO-ref matrix for T. If not, consider decreasing ChopT.)

The triple of angles defining U for the closest to MONO

In[1333]:=

```
{θ0, σ0, ϕ0}
```

Out[1333]=

```
{0., 0, 0.785398}
```

In[1334]:=

```
{θ0, σ0, ϕ0} / Degree
```

Out[1334]=

```
{0., 0, 45.}
```

The U for the closest to MONO

In[1335]:=

```
MatrixForm[Chop[UT[Tmat, Σ]]]
```

Out[1335]//MatrixForm=

$$\begin{pmatrix} 0.707107 & 0 & 0.707107 \\ 0 & 1. & 0 \\ -0.707107 & 0 & 0.707107 \end{pmatrix}$$

The distance to closest MONO

In[1336]:=

```
dT[Tmat, Σ]
```

Out[1336]=

6.94931×10^{-9}

The (chopped) angular distance to closest MONO

In[1337]:=

```
βT[Tmat, Σ] / Degree
```

Out[1337]=

```
0
```

The reference matrix

In[1338]:=

```
Ubar = MatrixUbar[UT[Tmat, Σ]];
Tref = Transpose[Ubar].Tmat.Ubar;
MatrixForm[Round[Tref, 0.001]]
```

Out[1340]//MatrixForm=

$$\begin{pmatrix} 2. & 0. & 0. & 0. & 0. & 0. \\ 0. & 2. & 0. & 0. & 0. & 0. \\ 0. & 0. & 3.25 & -0.433 & 0. & 0. \\ 0. & 0. & -0.433 & 3.75 & 0. & 0. \\ 0. & 0. & 0. & 0. & 5.5 & -0.5 \\ 0. & 0. & 0. & 0. & -0.5 & 5.5 \end{pmatrix}$$

The closest MONO map to Tmat.

Since the example Tmat has TET (and ORTH and MONO) symmetry, this closest-to-MONO will be the same as Tmat. For a TRIV map, this will provide something different from Tmat.

In[1341]:=

```
MatrixForm[Chop[Closest[Tmat, Σ]]]
```

Out[1341]//MatrixForm=

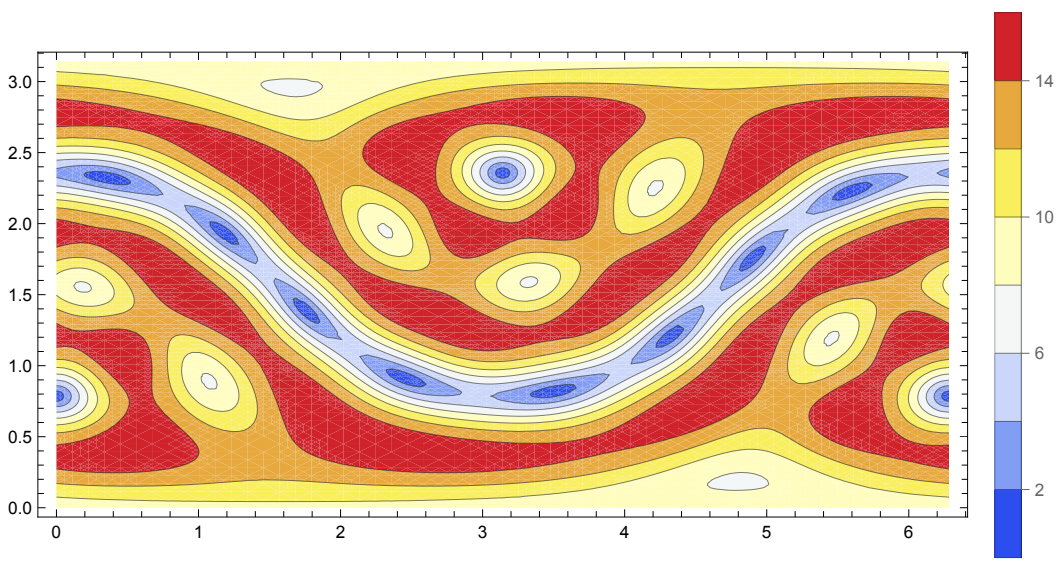
$$\begin{pmatrix} 2.625 & 0.153093 & -0.625 & 0.22964 & 0.132583 & 0 \\ 0.153093 & 5.0625 & -0.153093 & -0.65625 & -0.378886 & 0.433013 \\ -0.625 & -0.153093 & 2.625 & -0.22964 & -0.132583 & 0 \\ 0.22964 & -0.65625 & -0.22964 & 3.64062 & 0.947215 & -0.216506 \\ 0.132583 & -0.378886 & -0.132583 & 0.947215 & 2.54688 & -0.125 \\ 0 & 0.433013 & 0 & -0.216506 & -0.125 & 5.5 \end{pmatrix}$$

Plot the 2D function that represents the search over U (specifically θ and ϕ)
For the TET example, this plot will NOT appear above when running the OutputFor command (with WantDetails), since the plot is only produced when the distance is >0.

In[1342]:=

```
ContourPlot[Alpha[Tmat, {θ, ϕ}, MONO] / Degree, {θ, 0, 2 π},
 {ϕ, 0, π}, ColorFunction → (ColorData["TemperatureMap"]),
 PlotLegends → Automatic, AspectRatio → Automatic, ImageSize → 500]
```

Out[1342]=

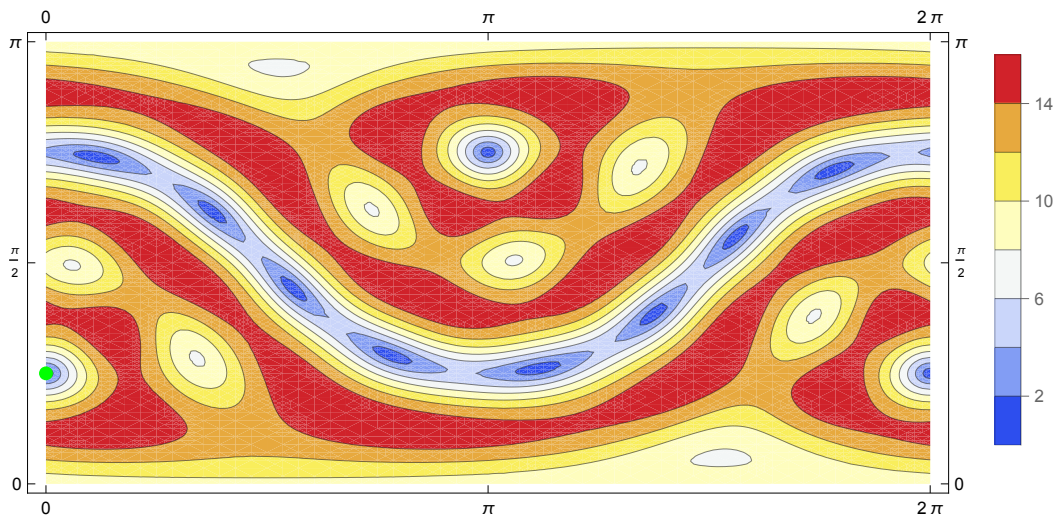


Now add the minimum as a green dot.
Here $\beta = 0$, since Tmat has TET (and ORTH and MONO) symmetry.

In[1343]:=

```
Show[{ContourPlot[Alpha[Tmat, {θ, ϕ}, MONO] / Degree, {θ, 0, 2 π}, {ϕ, 0, π},
    ColorFunction → (ColorData["TemperatureMap"]), PlotLegends → Automatic],
   Graphics[
    {PointSize[.015], {Green, Point[TPxyz0to2pi[UT[Tmat, MONO].{0, 0, 1}]]}}]}],
  FrameTicks → {Range[0, 2 π, π], Range[0, π, π / 2]}, AspectRatio → Automatic,
  PlotRange → All, ImageSize → 500]
```

Out[1343]=



Addendum 1b: output from OutputFor[Tmat, TET]

The example Tmat has symmetry TET.

In[1344]:=

```
Σ = TET;
```

In[1345]:=

```
Print["Tmat = ", MatrixForm[Tmat], " = ", MatrixForm[N[Tmat]]];
```

$$\text{Tmat} = \begin{pmatrix} \frac{21}{8} & \frac{\sqrt{\frac{3}{2}}}{8} & -\frac{5}{8} & \frac{3\sqrt{\frac{3}{2}}}{16} & \frac{3}{16\sqrt{2}} & 0 \\ \frac{\sqrt{\frac{3}{2}}}{8} & \frac{81}{16} & -\frac{\sqrt{\frac{3}{2}}}{8} & -\frac{21}{32} & -\frac{7\sqrt{3}}{32} & \frac{\sqrt{3}}{4} \\ -\frac{5}{8} & -\frac{\sqrt{\frac{3}{2}}}{8} & \frac{21}{8} & -\frac{3\sqrt{\frac{3}{2}}}{16} & -\frac{3}{16\sqrt{2}} & 0 \\ \frac{3\sqrt{\frac{3}{2}}}{16} & -\frac{21}{32} & -\frac{3\sqrt{\frac{3}{2}}}{16} & \frac{233}{64} & \frac{35\sqrt{3}}{64} & -\frac{\sqrt{3}}{8} \\ \frac{3}{16\sqrt{2}} & -\frac{7\sqrt{3}}{32} & -\frac{3}{16\sqrt{2}} & \frac{35\sqrt{3}}{64} & \frac{163}{64} & -\frac{1}{8} \\ 0 & \frac{\sqrt{3}}{4} & 0 & -\frac{\sqrt{3}}{8} & -\frac{1}{8} & \frac{11}{2} \end{pmatrix} =$$

$$\begin{pmatrix} 2.625 & 0.153093 & -0.625 & 0.22964 & 0.132583 & 0. \\ 0.153093 & 5.0625 & -0.153093 & -0.65625 & -0.378886 & 0.433013 \\ -0.625 & -0.153093 & 2.625 & -0.22964 & -0.132583 & 0. \\ 0.22964 & -0.65625 & -0.22964 & 3.64063 & 0.947215 & -0.216506 \\ 0.132583 & -0.378886 & -0.132583 & 0.947215 & 2.54688 & -0.125 \\ 0. & 0.433013 & 0. & -0.216506 & -0.125 & 5.5 \end{pmatrix}$$

In[1346]:=

```
OutputFor[Tmat, Σ]
```

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NMinimize = $\{8.82384\times10^{-8}, \{\theta\to3.14159, \sigma\to2.87979, \phi\to2.35619\}\}$

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{TET}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are $\{180., 165., 135.\}$)

$$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} -0.683013 & -0.183013 & -0.707107 \\ -0.258819 & 0.965926 & 0 \\ 0.683013 & 0.183013 & -0.707107 \end{pmatrix}$$ (A TET-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{TET}(U))$)

$\beta^T_{TET} = 0$ (Angle between T and $\mathcal{T}_{TET}$. The initial $\beta^T_{TET} = 9.1\times10^{-9}$ is here chopped to zero, since the chop threshold is set at 0.01°)

Since $\beta^T_{TET} = 0$, T is assigned symmetry at least TET.

$\mathcal{V}_{TET}(U_0)$ contains T

$d(T, \mathcal{T}_{TET}) = 8.8\times10^{-8}$ (Distance from T to $\mathcal{T}_{TET}$)

$$T_{TET} = [\overline{U_0}]^T[T][\overline{U_0}] = \begin{pmatrix} 2. & 0 & 0 & 0 & 0 & 0 \\ 0 & 2. & 0 & 0 & 0 & 0 \\ 0 & 0 & 3. & 0 & 0 & 0 \\ 0 & 0 & 0 & 4. & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.5 & -0.5 \\ 0 & 0 & 0 & 0 & -0.5 & 5.5 \end{pmatrix}$$ (Should be a TET-ref matrix for T. If not, consider decreasing ChopT.)

The triple of angles defining U for the closest to TET

In[1347]:=

```
{θ0, σ0, ϕ0}
```

Out[1347]=

```
{3.14159, 2.87979, 2.35619}
```

In[1348]:=

```
{θ0, σ0, ϕ0} / Degree
```

Out[1348]=

```
{180., 165., 135.}
```

The U for the closest to TET

In[1349]:=

```
MatrixForm[Chop[UT[Tmat, Σ], 10^-7]]
```

Out[1349]//MatrixForm=

$$\begin{pmatrix} -0.683013 & -0.183013 & -0.707107 \\ -0.258819 & 0.965926 & 0 \\ 0.683013 & 0.183013 & -0.707107 \end{pmatrix}$$

The distance to closest XISO

In[1350]:=

```
dT[Tmat, Σ]
```

Out[1350]=

8.82384×10^{-8}

The (chopped) angular distance to closest XISO

In[1351]:=

```
βT[Tmat, Σ] / Degree
```

Out[1351]=

```
0
```

The reference matrix

In[1352]:=

```
Ubar = MatrixUbar[UT[Tmat, Σ]];
Tref = Transpose[Ubar].Tmat.Ubar;
MatrixForm[Round[Tref, 0.001]]
```

Out[1354]//MatrixForm=

$$\begin{pmatrix} 2. & 0. & 0. & 0. & 0. & 0. \\ 0. & 2. & 0. & 0. & 0. & 0. \\ 0. & 0. & 3. & 0. & 0. & 0. \\ 0. & 0. & 0. & 4. & 0. & 0. \\ 0. & 0. & 0. & 0. & 5.5 & -0.5 \\ 0. & 0. & 0. & 0. & -0.5 & 5.5 \end{pmatrix}$$

Addendum 1c: output from OutputFor[Tmat, XISO]

The example Tmat does not have symmetry Σ.

In[1355]:=

```
Σ = XISO;
```

In[1356]:=

```
Print["Tmat = ", MatrixForm[Tmat], " = ", MatrixForm[N[Tmat]]];
```

$$\text{Tmat} = \begin{pmatrix} \frac{21}{8} & \frac{\sqrt{\frac{3}{2}}}{8} & -\frac{5}{8} & \frac{3\sqrt{\frac{3}{2}}}{16} & \frac{3}{16\sqrt{2}} & 0 \\ \frac{\sqrt{\frac{3}{2}}}{8} & \frac{81}{16} & -\frac{\sqrt{\frac{3}{2}}}{8} & -\frac{21}{32} & -\frac{7\sqrt{3}}{32} & \frac{\sqrt{3}}{4} \\ -\frac{5}{8} & -\frac{\sqrt{\frac{3}{2}}}{8} & \frac{21}{8} & -\frac{3\sqrt{\frac{3}{2}}}{16} & -\frac{3}{16\sqrt{2}} & 0 \\ \frac{3\sqrt{\frac{3}{2}}}{16} & -\frac{21}{32} & -\frac{3\sqrt{\frac{3}{2}}}{16} & \frac{233}{64} & \frac{35\sqrt{3}}{64} & -\frac{\sqrt{3}}{8} \\ \frac{3}{16\sqrt{2}} & -\frac{7\sqrt{3}}{32} & -\frac{3}{16\sqrt{2}} & \frac{35\sqrt{3}}{64} & \frac{163}{64} & -\frac{1}{8} \\ 0 & \frac{\sqrt{3}}{4} & 0 & -\frac{\sqrt{3}}{8} & -\frac{1}{8} & \frac{11}{2} \end{pmatrix} =$$

$$\begin{pmatrix} 2.625 & 0.153093 & -0.625 & 0.22964 & 0.132583 & 0. \\ 0.153093 & 5.0625 & -0.153093 & -0.65625 & -0.378886 & 0.433013 \\ -0.625 & -0.153093 & 2.625 & -0.22964 & -0.132583 & 0. \\ 0.22964 & -0.65625 & -0.22964 & 3.64063 & 0.947215 & -0.216506 \\ 0.132583 & -0.378886 & -0.132583 & 0.947215 & 2.54688 & -0.125 \\ 0. & 0.433013 & 0. & -0.216506 & -0.125 & 5.5 \end{pmatrix}$$

In[1357]:=

```
OutputFor[Tmat, Σ]
```

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NMinimize = $\{0.707107, \{\theta \to 3.14159, \sigma \to -2.36917, \phi \to 2.35619\}\}$

(minimizing the function $(\theta, \sigma, \phi) \longrightarrow d(T, \mathcal{V}_{XISO}(U))$, $U = \hat{U}_S(\theta,\sigma,\phi)$)

($(\theta_0, \sigma_0, \phi_0)$ in degrees are $\{180., 0., 135.\}$)

$$U_0 = \hat{U}_S(\theta_0,\sigma_0,\phi_0) = \begin{pmatrix} 0.707107 & 0 & -0.707107 \\ 0 & -1. & 0 \\ -0.707107 & 0 & -0.707107 \end{pmatrix}$$ (A XISO

-minimizer for T. It minimizes the function $U \longrightarrow d(T, \mathcal{V}_{XISO}(U))$)

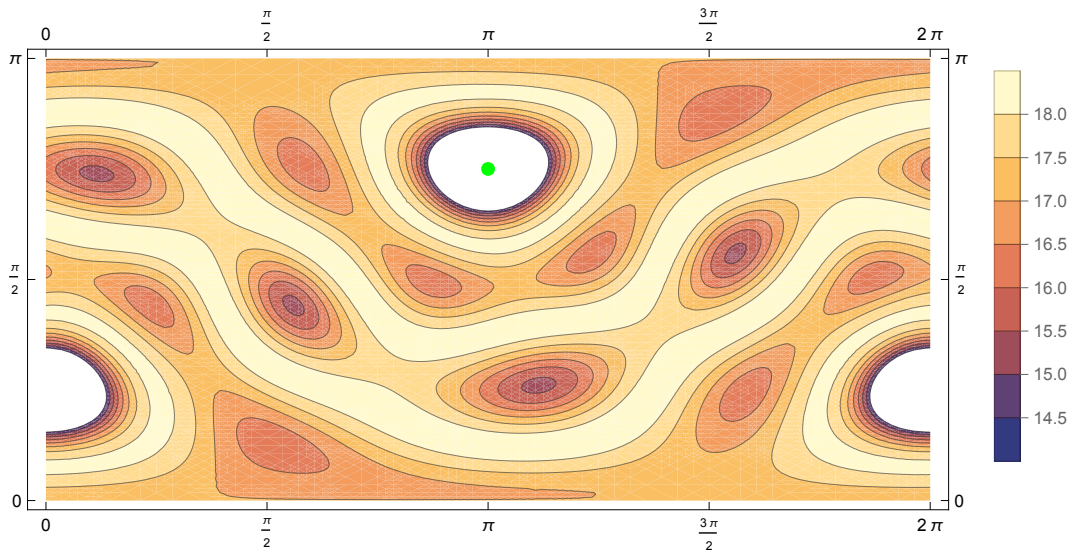
$\beta^{T}_{XISO} = 0.073 = 4.18^{\circ}$ (Angle between T and $\mathcal{T}_{XISO}$)

$\mathcal{V}_{XISO}(U_0)$ contains a closest map to T in $\mathcal{T}_{XISO}$

$d(T, \mathcal{T}_{XISO}) = 0.707$ (Distance from T to $\mathcal{T}_{XISO}$)

Does the green point look like a correct
GLOBAL minimum? If not, the minimization has failed.

Uniqueness (or not) of the closest XISO map is usually obvious from the contour plot.



$$P(T, \mathcal{V}_{XISO}(U_0)) = \begin{pmatrix} 2.75 & 0 & -0.75 & 0 & 0 & 0 \\ 0 & 5. & 0 & -0.75 & -0.433013 & 0.433013 \\ -0.75 & 0 & 2.75 & 0 & 0 & 0 \\ 0 & -0.75 & 0 & 3.5 & 0.866025 & -0.216506 \\ 0 & -0.433013 & 0 & 0.866025 & 2.5 & -0.125 \\ 0 & 0.433013 & 0 & -0.216506 & -0.125 & 5.5 \end{pmatrix}$$

(a closest elastic map to T having symmetry at least XISO)

The triple of angles defining U for the closest to XISO

In[1358]:=

```
{θ0, σ0, ϕ0}
```

Out[1358]=

{3.14159, 0, 2.35619}

In[1359]:=

```
{θ0, σ0, ϕ0} / Degree
```

Out[1359]=

```
{180., 0, 135.}
```

The U for the closest to XISO

In[1360]:=

```
MatrixForm[Chop[UT[Tmat, Σ]]]
```

Out[1360]//MatrixForm=

$$\begin{pmatrix} 0.707107 & 0 & -0.707107 \\ 0 & -1. & 0 \\ -0.707107 & 0 & -0.707107 \end{pmatrix}$$

The distance to closest XISO

In[1361]:=

```
dT[Tmat, Σ]
```

Out[1361]=

```
0.707107
```

The (chopped) angular distance to closest XISO

In[1362]:=

```
βT[Tmat, Σ] / Degree
```

Out[1362]=

```
4.18244
```

Closest XISO map to Tmat

In[1363]:=

```
MatrixForm[Chop[Closest[Tmat, Σ]]]
```

Out[1363]//MatrixForm=

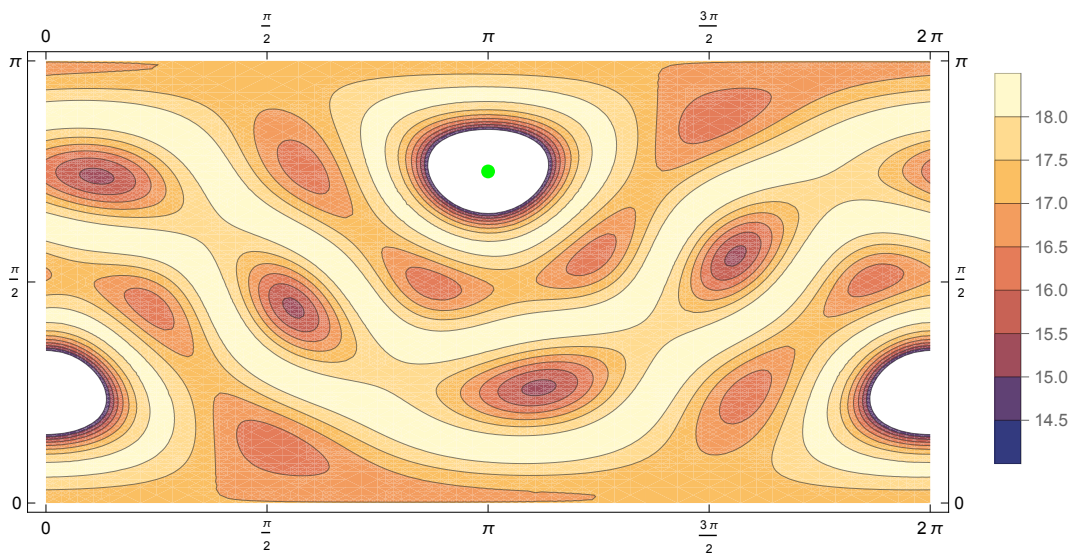
$$\begin{pmatrix} 2.75 & 0 & -0.75 & 0 & 0 & 0 \\ 0 & 5. & 0 & -0.75 & -0.433013 & 0.433013 \\ -0.75 & 0 & 2.75 & 0 & 0 & 0 \\ 0 & -0.75 & 0 & 3.5 & 0.866025 & -0.216506 \\ 0 & -0.433013 & 0 & 0.866025 & 2.5 & -0.125 \\ 0 & 0.433013 & 0 & -0.216506 & -0.125 & 5.5 \end{pmatrix}$$

Distance to closest XISO, with the global minimum plotted as a green point

In[1364]:=

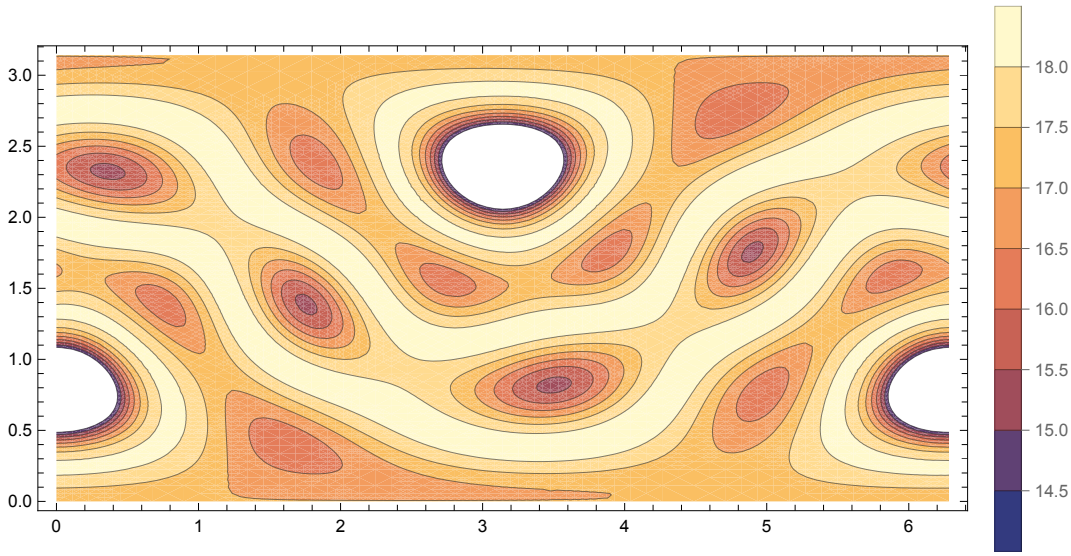
```
Show[{ContourPlot[Alpha[Tmat, {θ, ϕ}, XISO] / Degree,
    {θ, 0, 2 π}, {ϕ, 0, π}, PlotLegends → Automatic],
  Graphics[{PointSize[.015], Green, Point[TPxyz0to2pi[UT[Tmat, XISO].{0, 0, 1}]]}]},
 FrameTicks → {Range[0, 2 π, π / 2], Range[0, π, π / 2]},
 AspectRatio → Automatic, ImageSize → 500]
```

Out[1364]=



Contour plot but without the green dot

In[1365]:=

```
ContourPlot[Alpha[Tmat, {θ, ϕ}, XISO] / Degree, {θ, 0, 2 π}, {ϕ, 0, π},
 PlotLegends → Automatic, AspectRatio → Automatic, ImageSize → 500]
```

Out[1365]=