Optimization of the Cosine Weighted Linear B - spline Kernel

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For questions or concerns please contact the first author.

In[7]:=
```
ClearAll;
```

In[8]:=
```
Get["Bspline.m", Path → {"~/Desktop"}]
```

Start by defining the cosine weighted kernel

In[9]:=
```
b[t_] := Max[0, 1 - Abs[t]];
```

In[10]:=
```
l[x_, y_, z_] := b[x] b[ y ] b[z];
```

In[11]:=
```
w[x_, y_, z_] := 1/2 + 1/6 λ (Cos[2 Pi x] + Cos[2 Pi y] + Cos[2 Pi z]);
```

In[12]:=
```
basis[x_, y_, z_] := l[x / 2, y / 2, z / 2] w[x / 2, y / 2, z / 2]
```

Make sure the generator is normalized to have the same integral as the determinant of the lattice, i.e. 4

In[13]:=
```
Integrate[basis[x, y, z], {x, -2, 2}, {y, -2, 2}, {z, -2, 2}]
```

Out[13]= 4

In[14]:= **Evaluation of the Autocorrelation sequence in terms of λ**

Out[14]= Evaluation of the Autocorrelation sequence in terms of λ

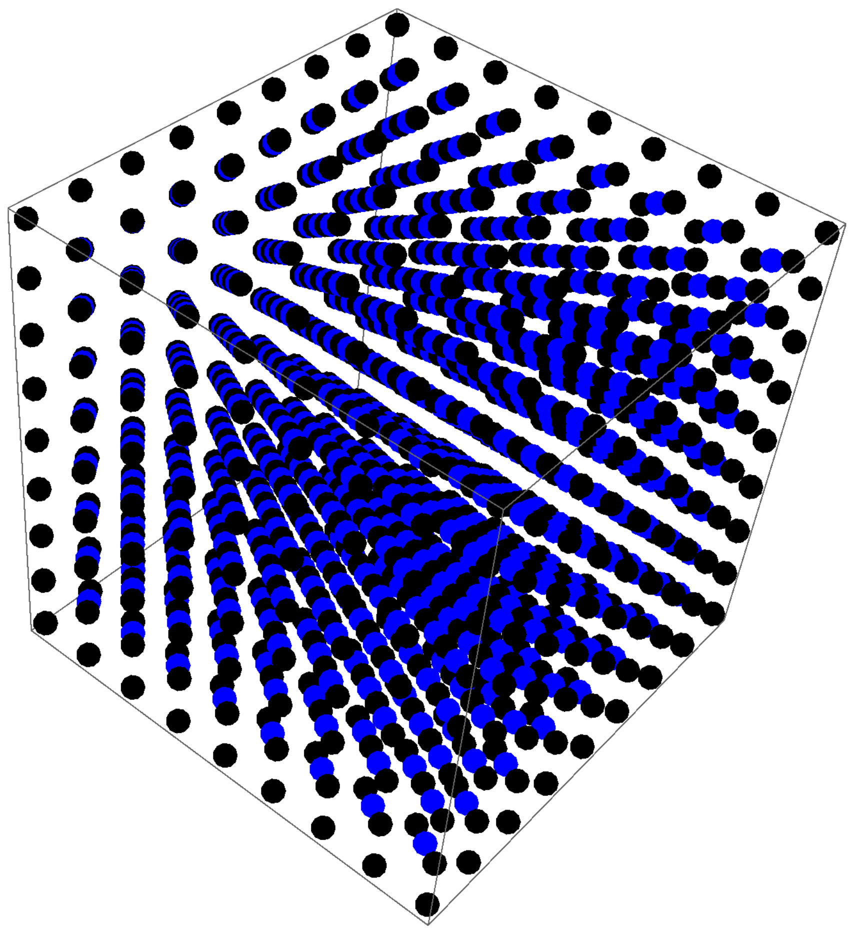
In[15]:=
```
M = {{2, 0, 0}, {0, 2, 0}, {0, 0, 2}};
```

In[16]:=
```
τ = {1, 1, 1};
```

In[17]:=
```
pgrid = M.# & /@ Tuples[{-4, -3, -2, -1, 0, 1, 2, 3, 4}, 3];
sgrid = M.# + τ & /@ Tuples[{-4, -3, -2, -1, 0, 1, 2, 3}, 3];
```

In[19]:=
```
Graphics3D[{PointSize[0.03], Black, Point[pgrid], Blue, Point[sgrid]}]
```

Out[19]=



In[20]:=
$$\text{ACl}[\text{n1\_}, \text{n2\_}, \text{n3\_}] := \text{Integrate}\Big[\text{l}[x/2, y/2, z/2]\, \text{w}[x/2, y/2, z/2]\, \text{l}\Big[\frac{\text{n1}-x}{2}, \frac{\text{n2}-y}{2}, \frac{\text{n3}-z}{2}\Big]\, \text{w}\Big[\frac{\text{n1}-x}{2}, \frac{\text{n2}-y}{2}, \frac{\text{n3}-z}{2}\Big], \{x, -4, 4\}, \{y, -4, 4\}, \{z, -4, 4\}\Big];$$

In[21]:=
```
Timing[Parallelize[pcoeffs = ACl[#[[1]], #[[2]], #[[3]]] & /@ pgrid]]
Timing[Parallelize[scoeffs = ACl[#[[1]], #[[2]], #[[3]]] & /@ sgrid]]
```

Out[21]= {33.576842, {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, 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, 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, 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, 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, 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, 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, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, $\frac{24\pi^4 - 144\pi^2\lambda + 144\lambda^2 - 3\pi^2\lambda^2 + 4\pi^4\lambda^2}{2592\pi^4}$,
$\frac{48\pi^2 - 144\lambda - 3\lambda^2 + 8\pi^2\lambda^2}{1296\pi^2}$, $\frac{24\pi^4 - 144\pi^2\lambda + 144\lambda^2 - 3\pi^2\lambda^2 + 4\pi^4\lambda^2}{2592\pi^4}$, 0, 0, 0, 0, 0,

$0, \frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2}, \frac{2\left(6\,\pi^4 - 9\,\lambda^2 + \pi^4\,\lambda^2\right)}{81\,\pi^4}, \frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2}, 0,$

$0, 0, 0, 0, 0, \frac{24\,\pi^4 - 144\,\pi^2\,\lambda + 144\,\lambda^2 - 3\,\pi^2\,\lambda^2 + 4\,\pi^4\,\lambda^2}{2592\,\pi^4}, \frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2},$

$\frac{24\,\pi^4 - 144\,\pi^2\,\lambda + 144\,\lambda^2 - 3\,\pi^2\,\lambda^2 + 4\,\pi^4\,\lambda^2}{2592\,\pi^4}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,$

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, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,

$\frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2}, \frac{2\left(6\,\pi^4 - 9\,\lambda^2 + \pi^4\,\lambda^2\right)}{81\,\pi^4}, \frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2},$

$0, 0, 0, 0, 0, 0, \frac{2\left(6\,\pi^4 - 9\,\lambda^2 + \pi^4\,\lambda^2\right)}{81\,\pi^4}, \frac{48\,\pi^4 + 144\,\pi^2\,\lambda + 72\,\lambda^2 + 3\,\pi^2\,\lambda^2 + 8\,\pi^4\,\lambda^2}{81\,\pi^4},$

$\frac{2\left(6\,\pi^4 - 9\,\lambda^2 + \pi^4\,\lambda^2\right)}{81\,\pi^4}, 0, 0, 0, 0, 0, 0, \frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2}, \frac{2\left(6\,\pi^4 - 9\,\lambda^2 + \pi^4\,\lambda^2\right)}{81\,\pi^4},$

$\frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,$

0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,

$0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, \frac{24\,\pi^4 - 144\,\pi^2\,\lambda + 144\,\lambda^2 - 3\,\pi^2\,\lambda^2 + 4\,\pi^4\,\lambda^2}{2592\,\pi^4},$

$\frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2}, \frac{24\,\pi^4 - 144\,\pi^2\,\lambda + 144\,\lambda^2 - 3\,\pi^2\,\lambda^2 + 4\,\pi^4\,\lambda^2}{2592\,\pi^4}, 0, 0, 0, 0, 0,$

$0, \frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2}, \frac{2\left(6\,\pi^4 - 9\,\lambda^2 + \pi^4\,\lambda^2\right)}{81\,\pi^4}, \frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2}, 0,$

$0, 0, 0, 0, 0, \frac{24\,\pi^4 - 144\,\pi^2\,\lambda + 144\,\lambda^2 - 3\,\pi^2\,\lambda^2 + 4\,\pi^4\,\lambda^2}{2592\,\pi^4}, \frac{48\,\pi^2 - 144\,\lambda - 3\,\lambda^2 + 8\,\pi^2\,\lambda^2}{1296\,\pi^2},$

$\frac{24\,\pi^4 - 144\,\pi^2\,\lambda + 144\,\lambda^2 - 3\,\pi^2\,\lambda^2 + 4\,\pi^4\,\lambda^2}{2592\,\pi^4}, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,$

0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 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,
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, 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, 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, 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, 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, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}}

Out[22]= {266.412003, {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, 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, 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, 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,

$0, 0, 0, 0, 0, \frac{6\,\pi^2 + 3\,\lambda^2 - \pi^2\,\lambda^2}{331\,776\,\pi^2}, \frac{138\,\pi^2 + 45\,\lambda^2 - 23\,\pi^2\,\lambda^2}{331\,776\,\pi^2}, \frac{138\,\pi^2 + 45\,\lambda^2 - 23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$

$\frac{6\,\pi^2 + 3\,\lambda^2 - \pi^2\,\lambda^2}{331\,776\,\pi^2}, 0, 0, 0, 0, \frac{138\,\pi^2 + 45\,\lambda^2 - 23\,\pi^2\,\lambda^2}{331\,776\,\pi^2}, -\frac{23\left(-138\,\pi^2 - 21\,\lambda^2 + 23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$

$$-\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,$$

$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$$

$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,\ \frac{6\,\pi^2+3\,\lambda^2-\pi^2\,\lambda^2}{331\,776\,\pi^2},\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$$

$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ \frac{6\,\pi^2+3\,\lambda^2-\pi^2\,\lambda^2}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,$$

$$0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$$

$$-\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$$

$$0,\ 0,\ 0,\ 0,\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{529\left(-138\,\pi^2+3\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$$

$$-\frac{529\left(-138\,\pi^2+3\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ 0,\ 0,$$

$$0,\ 0,\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{529\left(-138\,\pi^2+3\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$$

$$-\frac{529\left(-138\,\pi^2+3\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,$$

$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$$

$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,$$

$$0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$$

$$-\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$$

$$0,\ 0,\ 0,\ 0,\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{529\left(-138\,\pi^2+3\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$$

$$-\frac{529\left(-138\,\pi^2+3\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ 0,\ 0,$$

$$0,\ 0,\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{529\left(-138\,\pi^2+3\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$$

$$-\frac{529\left(-138\,\pi^2+3\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,$$

$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$$

$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,$$

$$0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ 0,\ \frac{6\,\pi^2+3\,\lambda^2-\pi^2\,\lambda^2}{331\,776\,\pi^2},\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$$

$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ \frac{6\,\pi^2+3\,\lambda^2-\pi^2\,\lambda^2}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$$
$$-\frac{23\,\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ -\frac{23\,\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},$$
$$0,\ 0,\ 0,\ 0,\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ -\frac{23\,\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},$$
$$-\frac{23\,\left(-138\,\pi^2-21\,\lambda^2+23\,\pi^2\,\lambda^2\right)}{331\,776\,\pi^2},\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,\ \frac{6\,\pi^2+3\,\lambda^2-\pi^2\,\lambda^2}{331\,776\,\pi^2},$$
$$\frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ \frac{138\,\pi^2+45\,\lambda^2-23\,\pi^2\,\lambda^2}{331\,776\,\pi^2},\ \frac{6\,\pi^2+3\,\lambda^2-\pi^2\,\lambda^2}{331\,776\,\pi^2},\ 0,\ 0,\ 0,\ 0,\ 0,$$

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, 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, 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, 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, 0, 0}}

Determine optimal λ by minimizing the error kernel

Fourier Transform of the generating function : We' ll use ordinary frequencies so that the reciprocal lattice is simply the inverse transpose (without the 2 Pi factor).

In[23]:=
```
S[u_] := Sinc[Pi u];
```

In[24]:=
$$\texttt{LF[u\_, v\_, w\_] :=} \frac{1}{2}\,S[u]^2\,S[v]^2\,S[w]^2+\frac{\lambda}{12}\,S[v]^2\,S[w]^2\,\left(S[u-1]^2+S[u+1]^2\right)+\frac{\lambda}{12}\,S[u]^2\,S[w]^2\,\left(S[v-1]^2+S[v+1]^2\right)+\frac{\lambda}{12}\,S[u]^2\,S[v]^2\,\left(S[w-1]^2+S[w+1]^2\right);$$

In[25]:=
```
ACLF[u_, v_, w_] = FullSimplify[MFseries[ MapThread[List, {pgrid, pcoeffs}], u, v, w] +
    MFseries[MapThread[List, {sgrid, scoeffs}], u, v, w]];
```

In[26]:=
```
Simplify[ACLF[0, 0, 0]]
```

Out[26]= 4

Finally, we can define the post - aliasing erroer kernel. The leading factors are needed since the kernel is not normlized.

In[27]:=
$$\texttt{Emin[u\_, v\_, w\_] :=} \frac{1}{4}\,\texttt{ACLF[2 Pi u, 2 Pi v, 2 Pi w]} - 4\,\texttt{LF[2 u, 2 v, 2 w]}^2$$

Verify that the generator is second order, i.e. all the terms up to order 4 in the Taylor expansion of Emin should be 0.

In[28]:=
```
Series[Emin[u, v, w], {u, 0, 3}, {v, 0, 3}, {w, 0, 3}]
```

Out[28]=
$$\left(O[w]^4+\left(\frac{32\,\lambda^2\,w^2}{9}+O[w]^4\right)v^2+O[v]^4\right)+\left(\left(\frac{32\,\lambda^2\,w^2}{9}+O[w]^4\right)+\left(\frac{32\,\lambda^2}{9}-\frac{256}{9}\left(\pi^2\,\lambda^2\right)w^2+O[w]^4\right)v^2+O[v]^4\right)u^2+O[u]^4$$

Collect all the 4 th order terms.

In[29]:=
```
orders = Select[Tuples[{0, 1, 2, 3, 4}, 3], Total[#] == 4 &]
```

Out[29]=
```
{{0, 0, 4}, {0, 1, 3}, {0, 2, 2}, {0, 3, 1}, {0, 4, 0}, {1, 0, 3}, {1, 1, 2}, {1, 2, 1},
 {1, 3, 0}, {2, 0, 2}, {2, 1, 1}, {2, 2, 0}, {3, 0, 1}, {3, 1, 0}, {4, 0, 0}}
```

In[30]:=
```
secondcoeffs =
 SeriesCoefficient[Emin[u, v, w], {u, 0, #[[1]]}, {v, 0, #[[2]]}, {w, 0, #[[3]]}] & /@
  orders
```

Out[30]=

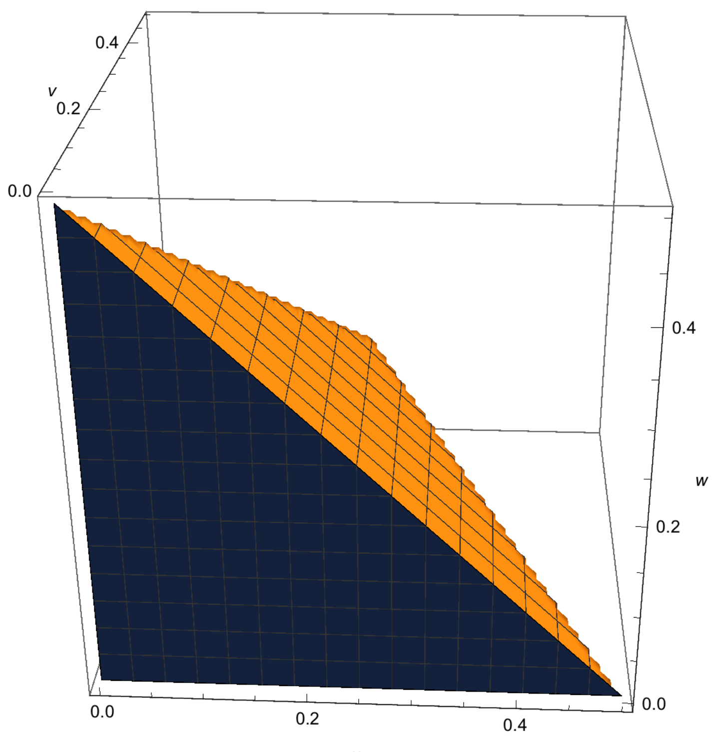
$$\left\{\frac{1}{90}\left(2\pi^4 - 2880\lambda + 320\pi^2\lambda - 160\lambda^2 + 10\pi^2\lambda^2 + 5\pi^4\lambda^2\right),\ 0,\ \frac{32\lambda^2}{9},\ 0,\ \frac{1}{90}\left(2\pi^4 - 2880\lambda + 320\pi^2\lambda - 160\lambda^2 + 10\pi^2\lambda^2 + 5\pi^4\lambda^2\right),\ 0,\ 0,\ 0,\ 0,\ \frac{32\lambda^2}{9},\ 0,\ \frac{32\lambda^2}{9},\ 0,\ 0,\ \frac{1}{90}\left(2\pi^4 - 2880\lambda + 320\pi^2\lambda - 160\lambda^2 + 10\pi^2\lambda^2 + 5\pi^4\lambda^2\right)\right\}$$

One octant of the rhombic dodecahedron (Voronoi cell of the dual FCC lattice)

In[31]:=
```
Region[u_, v_, w_] = Boole[
   (u + w - Pi < 0 && u + v - Pi < 0 && u > Pi/2) || (v + w - Pi < 0 && u + v - Pi < 0 && v > Pi/2) ||
    (u + w - Pi < 0 && w + v - Pi < 0 && w > Pi/2) || (0 ≤ u ≤ Pi/2 && 0 ≤ v ≤ Pi/2 && 0 ≤ w ≤ Pi/2)];
```

In[32]:=
```
RegionPlot3D[Region[2 Pi u, 2 Pi v, 2 Pi w] == 1 , {u, 0, 1 / 2},
 {v, 0, 1 / 2}, {w, 0, 1 / 2}, PlotPoints → 50, AxesLabel → {u, v, w}]
```

Out[32]=



In[33]:=
```
Minimize[Integrate[
  Region[2 Pi u, 2 Pi v, 2 Pi w] * ((u^#[[1]] v^#[[2]] w^#[[3]] & /@ orders).secondcoeffs),
  {u, 0, 1 / 2}, {v, 0, 1 / 2}, {w, 0, 1 / 2}], λ]
```

Out[33]=
$$\left\{\frac{1}{11\,059\,200}\left(54\pi^4+5\left(-\frac{416\left(7776-864\pi^2\right)^2}{\left(-416+54\pi^2+27\pi^4\right)^2}+\frac{54\pi^2\left(7776-864\pi^2\right)^2}{\left(-416+54\pi^2+27\pi^4\right)^2}+\frac{27\pi^4\left(7776-864\pi^2\right)^2}{\left(-416+54\pi^2+27\pi^4\right)^2}-\frac{15\,552\left(7776-864\pi^2\right)}{-416+54\pi^2+27\pi^4}+\frac{1728\pi^2\left(7776-864\pi^2\right)}{-416+54\pi^2+27\pi^4}\right)\right),\left\{\lambda\to\frac{7776-864\pi^2}{-416+54\pi^2+27\pi^4}\right\}\right\}$$

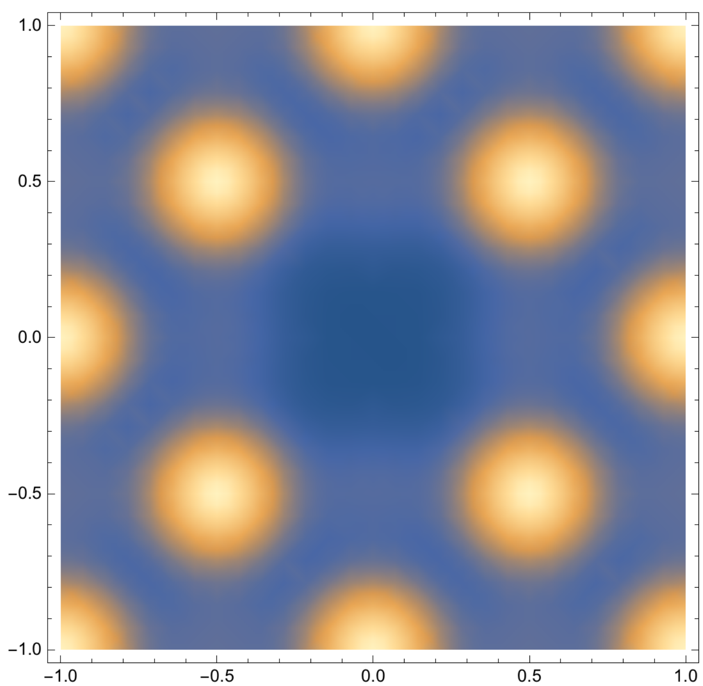
In[34]:= FullSimplify$\left[\frac{7776-864\pi^2}{-416+54\pi^2+27\pi^4}\right]$

Out[34]=
$$-\frac{864\left(-9+\pi^2\right)}{-416+27\pi^2\left(2+\pi^2\right)}$$

In[35]:= $\lambda_o = -\frac{864\left(-9+\pi^2\right)}{-416+27\pi^2\left(2+\pi^2\right)}$;

Comparison of how the error diminished with the optimized error kernel. We are only sowing the w = 0 slice.

In[36]:=
```
DensityPlot[Abs[Emin[u, v, 0]] /. λ → 1, {u, -1, 1}, {v, -1, 1}]
```

Out[36]=


In[37]:=
```
DensityPlot[Abs[Emin[u, v, 0]] /. λ → λo, {u, -1, 1}, {v, -1, 1}]
```

Out[37]=

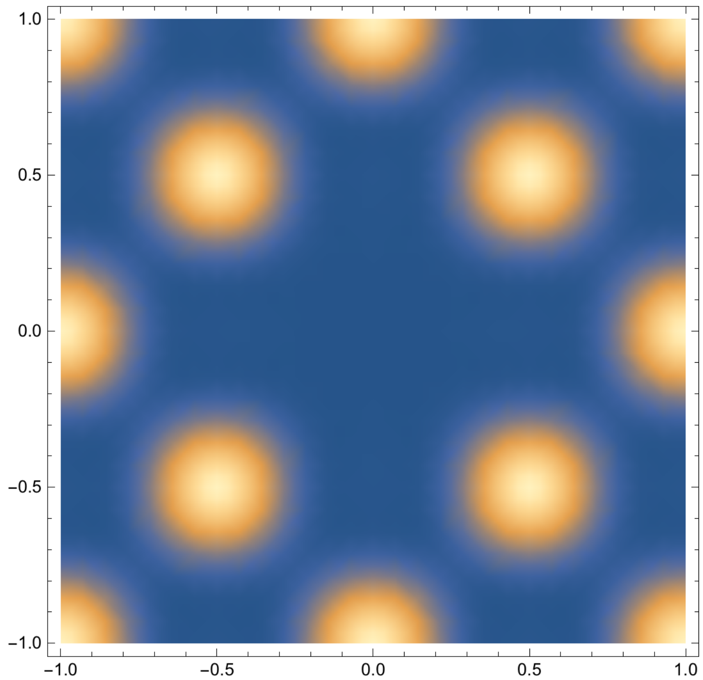


Figure out the gain in sampling rate as compared to trilinear interpolation

In[38]:=
```
ACTrilinear[u_, v_, w_] = FullSimplify[Fseries[{1 / 6, 2 / 3, 1 / 6}, 2 Pi u]
    Fseries[{1 / 6, 2 / 3, 1 / 6}, 2 Pi v] Fseries[{1 / 6, 2 / 3, 1 / 6}, 2 Pi w]]
```

Out[38]= $\frac{1}{27} (2 + \text{Cos}[2 \pi u]) (2 + \text{Cos}[2 \pi v]) (2 + \text{Cos}[2 \pi w])$

In[39]:=
```
EminTrilinear[u_, v_, w_] := ACTrilinear[u, v, w] - (S[u] S[v] S[w])^4
```

In[40]:=
```
Sqrt[NIntegrate[EminTrilinear[u, v, w] r^2 Sin[θ] /.
    {u → r Sin[θ] Cos[ϕ], v → r Sin[θ] Sin[ϕ], w → r Cos[θ]},
   {r, 0, 1 / 2}, {θ, 0, Pi}, {ϕ, 0, 2 Pi}]]
```

Out[40]= 0.126658

In[41]:=
```
Sqrt[Integrate[(((σ u)^#[[1]] (σ v)^#[[2]] (σ w)^#[[3]] & /@ orders).secondcoeffs) r^2 Sin[θ] /.
    {λ → λo, u → r Sin[θ] Cos[ϕ], v → r Sin[θ] Sin[ϕ], w → r Cos[θ]},
   {r, 0, 1 / 2}, {θ, 0, Pi}, {ϕ, 0, 2 Pi}]]
```

Out[41]=
$$\frac{1}{20 \left(-416 + 54 \pi^2 + 27 \pi^4\right)} \sqrt{\left(\frac{1}{42} \pi \left(3\,045\,703\,680 + \pi^2 \left(-979\,153\,920 + \pi^2 \left(-46\,206\,464 + 27 \pi^2 \left(1\,104\,256 + \pi^2 \left(-69\,844 + 27 \pi^2 \left(4 + \pi^2\right)\right)\right)\right)\right)\right)\right)} \sqrt{\sigma^4}$$

In[42]:=
$$\textbf{Solve}\left[\frac{1}{20\left(-416+54\pi^2+27\pi^4\right)}\sqrt{\left(\frac{1}{42}\pi\left(3\,045\,703\,680+\pi^2\left(-979\,153\,920+\pi^2\left(-46\,206\,464+27\pi^2\left(1\,104\,256+\pi^2\left(-69\,844+27\pi^2\left(4+\pi^2\right)\right)\right)\right)\right)\right)\right)}\sqrt{\sigma^4}==0.1266581207052528\grave{},\ \sigma\right]$$

Out[42]= $\{\{\sigma\to-1.01996\},\ \{\sigma\to0.\,-1.01996\,\mathrm{i}\},\ \{\sigma\to0.\,+1.01996\,\mathrm{i}\},\ \{\sigma\to1.01996\}\}$

The actual gain is obtained by multiplying σ by a normalization factor of $4^{-1/3}$.

Convolve to obtain downsampling filter that is to be applied to the fine scale CC grid before subsampling to BCC.

In[43]:=
```
DS[n1_, n2_, n3_] :=
  Integrate[l[x / 2, y / 2, z / 2] w[x / 2, y / 2, z / 2] l[n1 - x, n2 - y, n3 - z],
   {x, -3, 3}, {y, -3, 3}, {z, -3, 3}];

dsfilter = Table[DS[i, j, k], {i, -3, 3}, {j, -3, 3}, {k, -3, 3}];
```

In[45]:=
```
dsfilter
```

Out[45]=
$$\{\{\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\}\},$$
$$\{\{0,0,0,0,0,0,0\},\left\{0,\frac{1}{3456},\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{5\pi^2+8\lambda}{1728\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{1}{3456},0\right\},$$
$$\left\{0,\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},0\right\},$$
$$\left\{0,\frac{5\pi^2+8\lambda}{1728\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{5\left(5\pi^2+16\lambda\right)}{864\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{5\pi^2+8\lambda}{1728\pi^2},0\right\},$$
$$\left\{0,\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},0\right\},$$
$$\left\{0,\frac{1}{3456},\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{5\pi^2+8\lambda}{1728\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{1}{3456},0\right\},\{0,0,0,0,0,0,0\}\},$$
$$\{\{0,0,0,0,0,0,0\},\left\{0,\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},0\right\},$$
$$\left\{0,\frac{3\pi^2-8\lambda}{288\pi^2},\frac{\pi^2-4\lambda}{16\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{\pi^2-4\lambda}{16\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},0\right\},$$
$$\left\{0,\frac{15\pi^2+4\lambda}{864\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{5\left(15\pi^2+28\lambda\right)}{432\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},0\right\},$$
$$\left\{0,\frac{3\pi^2-8\lambda}{288\pi^2},\frac{\pi^2-4\lambda}{16\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{\pi^2-4\lambda}{16\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},0\right\},$$
$$\left\{0,\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},0\right\},\{0,0,0,0,0,0,0\}\},$$

$$\left\{\{0,0,0,0,0,0,0\},\left\{0,\frac{5\pi^2+8\lambda}{1728\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{5\left(5\pi^2+16\lambda\right)}{864\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{5\pi^2+8\lambda}{1728\pi^2},0\right\},\right.$$
$$\left\{0,\frac{15\pi^2+4\lambda}{864\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{5\left(15\pi^2+28\lambda\right)}{432\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},0\right\},$$
$$\left\{0,\frac{5\left(5\pi^2+16\lambda\right)}{864\pi^2},\frac{5\left(15\pi^2+28\lambda\right)}{432\pi^2},\frac{25\left(5\pi^2+24\lambda\right)}{432\pi^2},\frac{5\left(15\pi^2+28\lambda\right)}{432\pi^2},\frac{5\left(5\pi^2+16\lambda\right)}{864\pi^2},0\right\},$$
$$\left\{0,\frac{15\pi^2+4\lambda}{864\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{5\left(15\pi^2+28\lambda\right)}{432\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},0\right\},\left\{0,\frac{5\pi^2+8\lambda}{1728\pi^2},\right.$$
$$\left.\left.\frac{15\pi^2+4\lambda}{864\pi^2},\frac{5\left(5\pi^2+16\lambda\right)}{864\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{5\pi^2+8\lambda}{1728\pi^2},0\right\},\{0,0,0,0,0,0,0\}\right\},$$
$$\left\{\{0,0,0,0,0,0,0\},\left\{0,\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},0\right\},\right.$$
$$\left\{0,\frac{3\pi^2-8\lambda}{288\pi^2},\frac{\pi^2-4\lambda}{16\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{\pi^2-4\lambda}{16\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},0\right\},$$
$$\left\{0,\frac{15\pi^2+4\lambda}{864\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{5\left(15\pi^2+28\lambda\right)}{432\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},0\right\},$$
$$\left\{0,\frac{3\pi^2-8\lambda}{288\pi^2},\frac{\pi^2-4\lambda}{16\pi^2},\frac{15\pi^2-16\lambda}{144\pi^2},\frac{\pi^2-4\lambda}{16\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},0\right\},$$
$$\left.\left\{0,\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},0\right\},\{0,0,0,0,0,0,0\}\right\},$$
$$\left\{\{0,0,0,0,0,0,0\},\left\{0,\frac{1}{3456},\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{5\pi^2+8\lambda}{1728\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{1}{3456},0\right\},\right.$$
$$\left\{0,\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},0\right\},$$
$$\left\{0,\frac{5\pi^2+8\lambda}{1728\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{5\left(5\pi^2+16\lambda\right)}{864\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{5\pi^2+8\lambda}{1728\pi^2},0\right\},$$
$$\left\{0,\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{15\pi^2+4\lambda}{864\pi^2},\frac{3\pi^2-8\lambda}{288\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},0\right\},$$
$$\left.\left\{0,\frac{1}{3456},\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{5\pi^2+8\lambda}{1728\pi^2},\frac{3\pi^2-4\lambda}{1728\pi^2},\frac{1}{3456},0\right\},\{0,0,0,0,0,0,0\}\right\},$$
$$\{\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},$$
$$\left.\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\},\{0,0,0,0,0,0,0\}\}\right\}$$