Elementary tight – binding approach for simple electronic structure calculations – Applications to modeling coumarin based dyes for dye – sensitized solar cells

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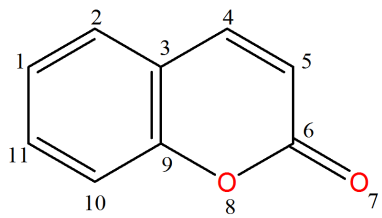
Supplementary materials

Example of calculation of the energy spectrum and molecular orbitals of basic coumarin.

Schematic molecular structure of the basic coumarin showing the atom numbering.



Steps in solving the problem.

Write the energy matrix row by row :

```
Hmat = {{x, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
  {1, x, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, x, 1, 0, 0, 0, 0, 0, 0, 0},
  {0, 0, 1, x, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, x, 1, 0, 0, 0, 0, 0},
  {0, 0, 0, 0, 1, x, 1, 0.8`, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 2 + x, 0, 0, 0, 0},
  {0, 0, 0, 0, 0, 0.8`, 0, 1 + x, 0.8`, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8`, x, 1, 0},
  {0, 0, 0, 0, 0, 0, 0, 0, 1, x, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, x}}
```

```
{{x, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, x, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, x, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, x, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, x, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, x, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 2 + x, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, 1 + x, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, x, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, x, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, x}}
```

Check the energy matrix :

```
MatrixForm[Hmat]
```

$$\begin{pmatrix} x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & x & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & x & 1 & 0.8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2+x & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.8 & 0 & 1+x & 0.8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.8 & x & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & x \end{pmatrix}$$

Calculate the determinant of the matrix :

```
Det[Hmat]
```

$$-6.12 + 3.88\,x + 50.6\,x^2 - 5.8\,x^3 - 113.4\,x^4 - 16.04\,x^5 + 87.92\,x^6 + 21.6\,x^7 - 27.56\,x^8 - 8.28\,x^9 + 3\,x^{10} + x^{11}$$

Solve the secular equation :

```
Solve[Det[Hmat] == 0, x]
```

```
{{x → -2.60675}, {x → -1.92543}, {x → -1.6931},
 {x → -1.48923}, {x → -0.819316}, {x → -0.513283}, {x → 0.372864},
 {x → 0.6903}, {x → 1.40354}, {x → 1.64303}, {x → 1.93737}}
```

Write the matrix using the first solution of the secular equation :

```
Hmat1 = Hmat /. x → -2.606752144274527`
```

```
{{-2.60675, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, -2.60675, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, -2.60675, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, -2.60675, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, -2.60675, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, -2.60675, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, -0.606752, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, -1.60675, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, -2.60675, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, -2.60675, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, -2.60675}}
```

Find the coefficients corresponding to the first solution of the secular equation :

```
Eigensystem[Hmat1]
```

```
{{-4.54412, -4.24978, -4.01029, -3.29705, -2.97962,
  -2.09347, -1.78744, -1.11753, -0.913649, -0.681322, -3.23736 × 10^-15},
 {{-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {0.308593, -0.0743993, -0.186353, 0.380582, -0.438956, 0.340635,
   -0.0935032, -0.0340185, -0.228245, 0.402228, -0.432628},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {-0.346627, -0.114213, 0.176539, 0.377119, 0.385076, 0.196346,
   -0.384409, 0.364671, 0.0266615, -0.252032, -0.401994},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {-0.390408, -0.360747, -0.304185, -0.22494, -0.128921, -0.0232888,
   0.312309, -0.285286, -0.306727, -0.362352, -0.390957},
  {0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232,
   0.78159, 0.290657, 0.109536, 0.0530078, 0.0286421}}}
```

Write the matrix using the second solution of the secular equation :

```
Hmat2 = Hmat /. x → -1.9254303259407655`
```

```
{{-1.92543, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, -1.92543, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, -1.92543, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, -1.92543, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, -1.92543, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, -1.92543, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 0.0745697, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, -0.92543, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, -1.92543, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, -1.92543, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, -1.92543}}
```

Find the coefficients corresponding to the second solution of the secular equation :

```
Eigensystem[Hmat2]
```

```
{{-3.8628, -3.56846, -3.32897, -2.61573, -2.29829,
  -1.41215, -1.10611, 0.681322, -0.436205, -0.232327, 3.88578 × 10^-14},
 {{-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {-0.308593, 0.0743993, 0.186353, -0.380582, 0.438956, -0.340635,
   0.0935032, 0.0340185, 0.228245, -0.402228, 0.432628},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232,
   0.78159, 0.290657, 0.109536, 0.0530078, 0.0286421},
  {0.346627, 0.114213, -0.176539, -0.377119, -0.385076, -0.196346,
   0.384409, -0.364671, -0.0266615, 0.252032, 0.401994},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {0.390408, 0.360747, 0.304185, 0.22494, 0.128921, 0.0232888,
   -0.312309, 0.285286, 0.306727, 0.362352, 0.390957}}}
```

Continue in a similar way with the other solutions of the secular equation :

```
Hmat3 = Hmat /. x → -1.6931029837256308`
```

```
{{-1.6931, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, -1.6931, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, -1.6931, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, -1.6931, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, -1.6931, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, -1.6931, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 0.306897, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, -0.693103, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, -1.6931, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, -1.6931, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, -1.6931}}
```

```
Eigensystem[Hmat3]
```

```
{{-3.63048, -3.33613, -3.09665, -2.3834, -2.06597,
  -1.17982, 0.913649, -0.873787, 0.232327, -0.203878, -4.20775 × 10^-14},
 {{-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {-0.308593, 0.0743993, 0.186353, -0.380582, 0.438956, -0.340635,
   0.0935032, 0.0340185, 0.228245, -0.402228, 0.432628},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232,
   0.78159, 0.290657, 0.109536, 0.0530078, 0.0286421},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {-0.390408, -0.360747, -0.304185, -0.22494, -0.128921, -0.0232888,
   0.312309, -0.285286, -0.306727, -0.362352, -0.390957},
  {-0.346627, -0.114213, 0.176539, 0.377119, 0.385076, 0.196346,
   -0.384409, 0.364671, 0.0266615, -0.252032, -0.401994},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513}}}
```

```
Hmat4 = Hmat /. x → -1.4892254386056922`
```

```
{{-1.48923, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, -1.48923, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, -1.48923, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, -1.48923, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, -1.48923, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, -1.48923, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 0.510775, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, -0.489225, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, -1.48923, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, -1.48923, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, -1.48923}}
```

```
Eigensystem[Hmat4]
```

```
{{-3.4266, -3.13226, -2.89277, -2.17953, -1.86209,
  1.11753, -0.975943, -0.66991, 0.436205, 0.203878, -3.10862 × 10^-15},
 {{-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {-0.308593, 0.0743993, 0.186353, -0.380582, 0.438956, -0.340635,
   0.0935032, 0.0340185, 0.228245, -0.402228, 0.432628},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264, 0.106471,
   0.365923, -0.375312, -0.152798, 0.432285}, {0.021655, 0.027807, 0.0508311,
   0.104697, 0.222088, 0.474232, 0.78159, 0.290657, 0.109536, 0.0530078, 0.0286421},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {-0.390408, -0.360747, -0.304185, -0.22494, -0.128921, -0.0232888,
   0.312309, -0.285286, -0.306727, -0.362352, -0.390957},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {-0.346627, -0.114213, 0.176539, 0.377119, 0.385076, 0.196346,
   -0.384409, 0.364671, 0.0266615, -0.252032, -0.401994}}}
```

```
Hmat5 = Hmat /. x → -0.819315558180011`
```

```
{{-0.819316, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, -0.819316, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, -0.819316, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, -0.819316, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, -0.819316, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, -0.819316, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 1.18068, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, 0.180684, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, -0.819316, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, -0.819316, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, -0.819316}}
```

```
Eigensystem[Hmat5]
```

```
{{-2.75669, -2.46235, -2.22286, 1.78744, -1.50962,
  -1.19218, 1.10611, 0.873787, 0.66991, -0.306033, -2.22045 × 10^-16},
 {{-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {0.308593, -0.0743993, -0.186353, 0.380582, -0.438956, 0.340635,
   -0.0935032, -0.0340185, -0.228245, 0.402228, -0.432628},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232, 0.78159, 0.290657,
   0.109536, 0.0530078, 0.0286421}, {0.437847, -0.0953142, -0.372052, 0.352141,
   0.128969, -0.441168, 0.163985, 0.0144812, 0.410572, -0.295002, -0.206932},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {-0.390408, -0.360747, -0.304185, -0.22494, -0.128921, -0.0232888,
   0.312309, -0.285286, -0.306727, -0.362352, -0.390957},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {0.346627, 0.114213, -0.176539, -0.377119, -0.385076, -0.196346,
   0.384409, -0.364671, -0.0266615, 0.252032, 0.401994},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958}}}
```

```
Hmat6 = Hmat /. x → -0.5132826091824044`
```

```
{{-0.513283, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, -0.513283, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, -0.513283, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, -0.513283, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, -0.513283, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, -0.513283, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 1.48672, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, 0.486717, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, -0.513283, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, -0.513283, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, -0.513283}}
```

```
Eigensystem[Hmat6]
```

```
{{-2.45066, -2.15631, 2.09347, -1.91683,
  1.41215, -1.20358, 1.17982, 0.975943, -0.886146, 0.306033, 0.},
 {{-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {-0.308593, 0.0743993, 0.186353, -0.380582, 0.438956, -0.340635, 0.0935032,
   0.0340185, 0.228245, -0.402228, 0.432628}, {0.021655, 0.027807, 0.0508311,
   0.104697, 0.222088, 0.474232, 0.78159, 0.290657, 0.109536, 0.0530078, 0.0286421},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {-0.390408, -0.360747, -0.304185, -0.22494, -0.128921, -0.0232888,
   0.312309, -0.285286, -0.306727, -0.362352, -0.390957},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {-0.346627, -0.114213, 0.176539, 0.377119, 0.385076, 0.196346,
   -0.384409, 0.364671, 0.0266615, -0.252032, -0.401994},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111}}}
```

```
Hmat7 = Hmat /. x → 0.37286386948058353`
```

```
{{0.372864, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, 0.372864, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, 0.372864, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, 0.372864, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, 0.372864, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, 0.372864, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 2.37286, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, 1.37286, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, 0.372864, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, 0.372864, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0.372864}}
```

```
Eigensystem[Hmat7]
```

```
{{2.97962, 2.29829, 2.06597, 1.86209, -1.56451,
  -1.27017, 1.19218, -1.03068, 0.886146, -0.317436, 0.},
 {{0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232, 0.78159, 0.290657,
   0.109536, 0.0530078, 0.0286421}, {0.390408, 0.360747, 0.304185, 0.22494,
   0.128921, 0.0232888, -0.312309, 0.285286, 0.306727, 0.362352, 0.390957},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {-0.346627, -0.114213, 0.176539, 0.377119, 0.385076, 0.196346,
   -0.384409, 0.364671, 0.0266615, -0.252032, -0.401994},
  {-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {0.308593, -0.0743993, -0.186353, 0.380582, -0.438956, 0.340635,
   -0.0935032, -0.0340185, -0.228245, 0.402228, -0.432628},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285}}}
```

```
Hmat8 = Hmat /. x → 0.6902996943456455`
```

```
{{0.6903, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, 0.6903, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, 0.6903, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, 0.6903, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, 0.6903, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, 0.6903, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 2.6903, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, 1.6903, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, 0.6903, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, 0.6903, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0.6903}}
```

```
Eigensystem[Hmat8]
```

```
{{3.29705, 2.61573, 2.3834, 2.17953, 1.50962, -1.24707,
  1.20358, -0.952731, -0.713243, 0.317436, -8.88178 × 10^-16},
 {{0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232, 0.78159, 0.290657,
   0.109536, 0.0530078, 0.0286421}, {0.390408, 0.360747, 0.304185, 0.22494,
   0.128921, 0.0232888, -0.312309, 0.285286, 0.306727, 0.362352, 0.390957},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {-0.346627, -0.114213, 0.176539, 0.377119, 0.385076, 0.196346,
   -0.384409, 0.364671, 0.0266615, -0.252032, -0.401994},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {-0.308593, 0.0743993, 0.186353, -0.380582, 0.438956, -0.340635,
   0.0935032, 0.0340185, 0.228245, -0.402228, 0.432628},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932}}}
```

```
Hmat9 = Hmat /. x → 1.4035425762509315`
```

```
{{1.40354, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, 1.40354, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, 1.40354, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, 1.40354, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, 1.40354, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, 1.40354, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 3.40354, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, 2.40354, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, 1.40354, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, 1.40354, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1.40354}}
```

```
Eigensystem[Hmat9]
```

```
{{4.01029, 3.32897, 3.09665, 2.89277, 2.22286,
  1.91683, 1.03068, 0.713243, -0.53383, -0.239488, 2.66454 × 10^-15},
 {{0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232, 0.78159, 0.290657,
   0.109536, 0.0530078, 0.0286421}, {-0.390408, -0.360747, -0.304185, -0.22494,
   -0.128921, -0.0232888, 0.312309, -0.285286, -0.306727, -0.362352, -0.390957},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {-0.346627, -0.114213, 0.176539, 0.377119, 0.385076, 0.196346,
   -0.384409, 0.364671, 0.0266615, -0.252032, -0.401994},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {0.308593, -0.0743993, -0.186353, 0.380582, -0.438956, 0.340635,
   -0.0935032, -0.0340185, -0.228245, 0.402228, -0.432628},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247}}}
```

```
Hmat10 = Hmat /. x → 1.6430302223814772`
```

```
{{1.64303, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, 1.64303, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, 1.64303, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, 1.64303, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, 1.64303, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, 1.64303, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 3.64303, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, 2.64303, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, 1.64303, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, 1.64303, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1.64303}}
```

```
Eigensystem[Hmat10]
```

```
{{4.24978, 3.56846, 3.33613, 3.13226, 2.46235,
  2.15631, 1.27017, 0.952731, -0.294342, 0.239488, -3.55271×10^-15},
 {{0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232, 0.78159, 0.290657,
   0.109536, 0.0530078, 0.0286421}, {0.390408, 0.360747, 0.304185, 0.22494,
   0.128921, 0.0232888, -0.312309, 0.285286, 0.306727, 0.362352, 0.390957},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {0.346627, 0.114213, -0.176539, -0.377119, -0.385076, -0.196346,
   0.384409, -0.364671, -0.0266615, 0.252032, 0.401994},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {-0.308593, 0.0743993, 0.186353, -0.380582, 0.438956, -0.340635,
   0.0935032, 0.0340185, 0.228245, -0.402228, 0.432628}}}
```

```
Hmat11 = Hmat /. x → 1.937372697450384`
```

```
{{1.93737, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1},
 {1, 1.93737, 1, 0, 0, 0, 0, 0, 0, 0, 0}, {0, 1, 1.93737, 1, 0, 0, 0, 0, 0, 0, 0},
 {0, 0, 1, 1.93737, 1, 0, 0, 0, 0, 0, 0}, {0, 0, 0, 1, 1.93737, 1, 0, 0, 0, 0, 0},
 {0, 0, 0, 0, 1, 1.93737, 1, 0.8, 0, 0, 0}, {0, 0, 0, 0, 0, 1, 3.93737, 0, 0, 0, 0},
 {0, 0, 0, 0, 0, 0.8, 0, 2.93737, 0.8, 0, 0}, {0, 0, 0, 0, 0, 0, 0, 0.8, 1.93737, 1, 0},
 {0, 0, 0, 0, 0, 0, 0, 0, 1, 1.93737, 1}, {1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1.93737}}
```

```
Eigensystem[Hmat11]
```

```
{{4.54412, 3.8628, 3.63048, 3.4266, 2.75669,
  2.45066, 1.56451, 1.24707, 0.53383, 0.294342, -1.77636 × 10^-15},
 {{0.021655, 0.027807, 0.0508311, 0.104697, 0.222088, 0.474232, 0.78159, 0.290657,
   0.109536, 0.0530078, 0.0286421}, {-0.390408, -0.360747, -0.304185, -0.22494,
   -0.128921, -0.0232888, 0.312309, -0.285286, -0.306727, -0.362352, -0.390957},
  {0.179246, 0.352634, 0.417799, 0.354743, 0.182817, -0.0452144,
   0.147327, -0.508372, -0.395228, -0.262464, -0.0491513},
  {0.346627, 0.114213, -0.176539, -0.377119, -0.385076, -0.196346,
   0.384409, -0.364671, -0.0266615, 0.252032, 0.401994},
  {0.201664, 0.440185, 0.158986, -0.309925, -0.412913, -0.0283805,
   0.0240373, 0.457029, -0.074842, -0.426942, -0.274958},
  {0.408885, -0.0512373, -0.435184, -0.172135, 0.34683, 0.350157,
   -0.235523, 0.0855286, -0.402192, -0.274861, 0.261111},
  {-0.00838574, -0.429158, 0.168403, 0.366367, -0.305008, -0.25264,
   0.106471, 0.365923, -0.375312, -0.152798, 0.432285},
  {-0.437847, 0.0953142, 0.372052, -0.352141, -0.128969, 0.441168,
   -0.163985, -0.0144812, -0.410572, 0.295002, 0.206932},
  {0.233408, -0.418122, 0.353445, -0.0779525, -0.244035, 0.420466,
   -0.123538, -0.278212, 0.415401, -0.360463, 0.0905247},
  {-0.308593, 0.0743993, 0.186353, -0.380582, 0.438956, -0.340635,
   0.0935032, 0.0340185, 0.228245, -0.402228, 0.432628},
  {-0.381429, 0.402097, -0.397582, 0.368168, -0.315697, 0.243454,
   -0.0618316, -0.117666, 0.188582, -0.271221, 0.336874}}}
```