

Theory Computing Project Notebook

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Week 3 - Matrix methods:

Task 1: Simple Matrices:

$$Av = \lambda v$$

Now it is your turn. Use the built in functions to find the Eigenvectors and Eigenvalues of the matrix below

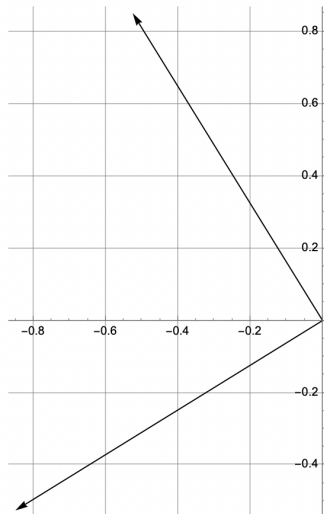
```
In[66]:= myNewMatrix = {{2.0, -1.0}, {-1.0, 3.0}};
myNewMatrix // MatrixForm
Out[67]/MatrixForm=

$$\begin{pmatrix} 2. & -1. \\ -1. & 3. \end{pmatrix}$$

eigenVecs = Eigenvectors[myNewMatrix]
eigenVals = Eigenvalues[myNewMatrix]
Out[75]= {{-0.525731, 0.850651}, {-0.850651, -0.525731}}
Out[76]= {3.61803, 1.38197}
```

Now plot those eigenvectors. Apply the matrix to the eigenvectors and see the eigenvalues make sense

```
In[83]:= Graphics[{Arrow[{0, 0}, eigenVecs[[1]]], Arrow[{0, 0}, eigenVecs[[2]]]}, Axes -> True, GridLines -> Automatic]
Out[83]=
```



```
In[106]:= leftMatrix = myNewMatrix.eigenVecs[[1]]
rightMatrix = eigenVals[[1]] * eigenVecs[[1]]
leftMatrix == rightMatrix
Out[106]= {-1.90211, 3.07768}
Out[107]= {-1.90211, 3.07768}
Out[108]= True
```

We know that applying the matrix A to an eigenvector scales it by its eigenvalue:

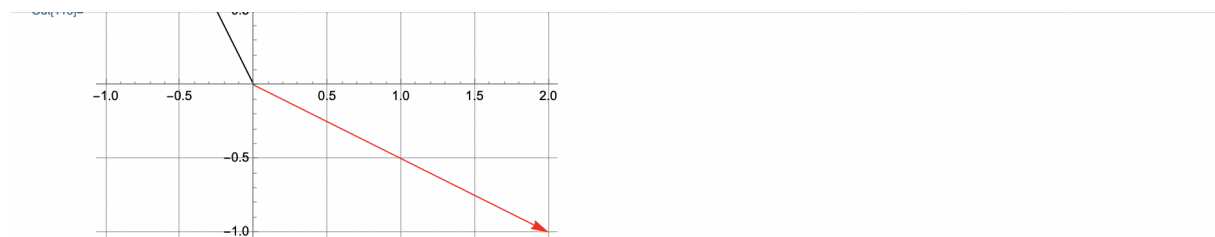
$$Av_i = \lambda_i v_i$$

Thus,

$$A \cdot \text{myNewVector} = A \cdot (av_1 + bv_2)$$

Since $Av_i = \lambda_i v_i$, this simplifies to:

$$A \cdot \text{myNewVector} = a\lambda_1 v_1 + b\lambda_2 v_2$$



We see that this vector changes direction under this matrix multiplication, and so is definitely not an eigenvector itself

```
In[116]:= coeffs = Solve[myNewVector == a * eigenVecs[[1]] + b * eigenVecs[[2]]
           |解方程
myNewVector // MatrixForm
           |矩阵格式
a * eigenVecs[[1]] + b * eigenVecs[[2]] /. coeffs // MatrixForm
           |矩阵格式

Out[116]:= {{a -> 2.22703, b -> -0.200811}}
```

```
Out[117]//MatrixForm=
  ( -1. )
  (  2. )
```

```
Out[118]//MatrixForm=
  ( -1.  2. )
```

The important realisation here is that by understanding the decomposition of any vector into eigenvectors, can understand the effect of the matrix on it. Stated another way, eigenvalues and eigenvectors contain all necessary information about the matrix. Try finding the result of matrix on vector above by using its eigen decomposition

```
In[120]:= newVector = coeffs[[1, 1, 2]] * eigenVals[[1]] * eigenVecs[[1]] + coeffs[[1, 2, 2]] * eigenVals[[2]] * eigenVecs[[2]]
directResult = myNewMatrix.myNewVector;
newVector == directResult

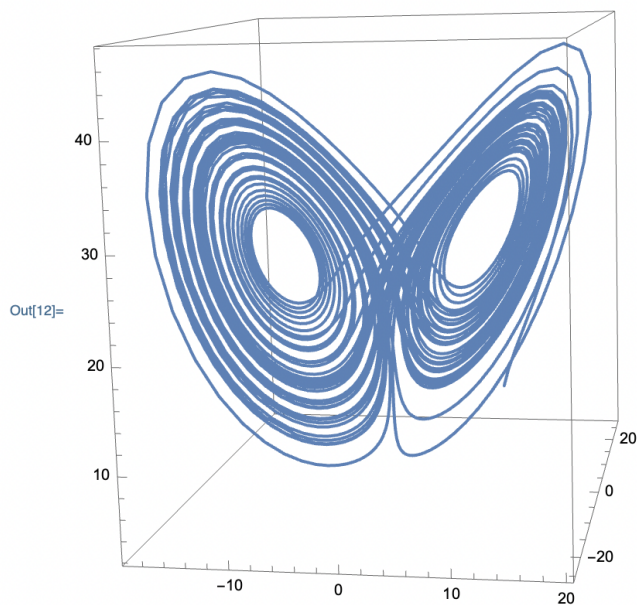
Out[120]:= {-4., 7.}
```

```
Out[122]:= True
```

Task 2: Simple ODE:

For cases with no analytic solution we can use a numerical solution NDSolve

```
In[7]:= (*Code 'borrowed' and slightly adapted from Wikipedia*)
tend = 50;
eq = {x'[t] ==  $\sigma$  (y[t] - x[t]), y'[t] == x[t] ( $\rho$  - z[t]) - y[t], z'[t] == x[t] y[t] -  $\beta$  z[t]};
init = {x[0] == 10, y[0] == 10, z[0] == 10};
pars = { $\sigma$  → 10,  $\rho$  → 28,  $\beta$  → 8/3};
Sols = NDSolve[eq /. pars, init], {x, y, z}, {t, 0, tend}][[1]];
      数值求解微分方程组
ParametricPlot3D[{x[t], y[t], z[t]} /. Sols, {t, 0, tend}]
      绘制三维参数图
```



Task 3: Springs Masses:

We are interested in transforming our equations into the eigenbasis. Thankfully eigenanalysis is easy in Mathematica.

```
In[18]:= Eigsys = Eigensystem[ODEmatrix]
```

[特征系统]

```
Out[18]:= {{-3 k/m, -k/m, 0}, {{1, -2, 1}, {-1, 0, 1}, {1, 1, 1}}}
```

Make sure you can qualitatively explain the three eigenstates with their respective eigenvalue. Remember that the eigenvalues will be associated with the frequency of oscillation.

Construct the transformation matrices discussed in the notes. Remember that the *columns* of TmatrixInv should be the eigenvectors.

```
In[19]:= TmatrixInv = Transpose[Eigsys[[2]]];
```

[转置]

```
Tmatrix = Inverse[TmatrixInv];
```

[逆]

```
Tmatrix // MatrixForm
```

[矩阵格式]

```
TmatrixInv // MatrixForm
```

[矩阵格式]

```
Out[21]//MatrixForm=
```

$$\begin{pmatrix} \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \\ -\frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

```
Out[22]//MatrixForm=
```

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

Essentially T will map our physical coordinates (x1, x2, x3) into the eigenstates, or normal modes (y1, y2, y3). T^{-1} does the opposite.

Show that T acting on X=(1,-2,1) indeed gives purely the first eigenstate. Similarly, show that the state Y=(0,1,0) gives X=(-1,0,1)

```
In[23]:= X1 = {1, -2, 1};
```

```
Y1 = Tmatrix.X1;
```

```
Y1 // MatrixForm
```

[矩阵格式]

```
Out[25]//MatrixForm=
```

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

```
In[26]:= Y2 = {0, 1, 0};
```

```
X2 = TmatrixInv.Y2;
```

```
X2 // MatrixForm
```

[矩阵格式]

```
Out[28]//MatrixForm=
```

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

Use the results above to construct the matrix
from $\mathbf{Q}\mathbf{T}^{-1}$ where \mathbf{Q} is the original ODE matrix.
Show it is the same as the diagonal matrix of eigenvalues

```
In[34]:= diagonalmatrix = Tmatrix.ODEmatrix.TmatrixInv;
diagonalmatrix // MatrixForm
```

矩阵格式

Out[35]/MatrixForm=

$$\begin{pmatrix} -\frac{3k}{m} & 0 & 0 \\ 0 & -\frac{k}{m} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

```
In[31]:= eigenVals = Eigsys[[1]]
DiagonalMatrixOfEig = DiagonalMatrix[eigenVals];
DiagonalMatrixOfEig // MatrixForm
```

对角矩阵

矩阵格式

Out[31]= $\left\{ -\frac{3k}{m}, -\frac{k}{m}, 0 \right\}$

Out[33]/MatrixForm=

$$\begin{pmatrix} -\frac{3k}{m} & 0 & 0 \\ 0 & -\frac{k}{m} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Let's print out each set of ODEs to show the reduction of complexity. Note however that even in the second case it would be simpler labelling as $y_i[t]$ rather than $xi[t]$

```
In[37]:= For[i = 1, i ≤ Length[Statevec], i += 1,
For循环 长度
Print[D[Statevec[[i]], {t, 2}] == (ODEmatrix.Statevec)[[i]] + AVEC[[i]]
打印 偏导
]
```

$$x1''[t] == -\frac{a k}{m} - \frac{k x1[t]}{m} + \frac{k x2[t]}{m}$$

$$x2''[t] == \frac{k x1[t]}{m} - \frac{2 k x2[t]}{m} + \frac{k x3[t]}{m}$$

$$x3''[t] == \frac{a k}{m} + \frac{k x2[t]}{m} - \frac{k x3[t]}{m}$$

```
In[36]:= For[i = 1, i ≤ Length[Statevec], i += 1,
For循环 长度
Print[D[(Tmatrix.Statevec)[[i]], {t, 2}] ==
打印 偏导
((Tmatrix.ODEmatrix.TmatrixInv).(Tmatrix.Statevec)[[i]] + (Tmatrix.Avec)[[i]])
]
```

$$\frac{x1''[t]}{6} - \frac{x2''[t]}{3} + \frac{x3''[t]}{6} == -\frac{3k \left(\frac{x1[t]}{6} - \frac{x2[t]}{3} + \frac{x3[t]}{6} \right)}{m}$$

$$-\frac{1}{2} x1''[t] + \frac{x3''[t]}{2} == \frac{a k}{m} - \frac{k \left(-\frac{x1[t]}{2} + \frac{x3[t]}{2} \right)}{m}$$

$$\frac{x1''[t]}{3} + \frac{x2''[t]}{3} + \frac{x3''[t]}{3} == 0$$

While the second form is clearly simpler due to its decoupling of equations, we will follow from the notes with $\ddot{y}_i = \lambda_i y_i + b_i$ (this is equivalent to what is written above)

```
In[38]:= Bvec = Tmatrix.Avec;
Bvec // MatrixForm
|矩阵格式

Out[39]//MatrixForm=

$$\begin{pmatrix} 0 \\ \frac{a k}{m} \\ 0 \end{pmatrix}$$


In[40]:= Print[DSolve[y1''[t] == Eigsys[[1]][[1]]*y1[t] + Bvec[[1]], y1[t], t]]
|打印 |求解微分方程


$$\left\{ \left\{ y1[t] \rightarrow c_1 \cos\left[\frac{\sqrt{3} \sqrt{k} t}{\sqrt{m}}\right] + c_2 \sin\left[\frac{\sqrt{3} \sqrt{k} t}{\sqrt{m}}\right] \right\} \right\}$$

```

Now solve the other equations

```
In[41]:= For[i = 1, i <= Length[Statevec], i += 1,
|For循环 |长度
Print[DSolve[y''[t] == Eigsys[[1]][[i]]*y[t] + Bvec[[i]], y[t], t] /.
|打印 |求解微分方程
y -> ToExpression["y" <> ToString[i]]
|转换为表达式 |转换为字符串
]


$$\left\{ \left\{ y1[t] \rightarrow c_1 \cos\left[\frac{\sqrt{3} \sqrt{k} t}{\sqrt{m}}\right] + c_2 \sin\left[\frac{\sqrt{3} \sqrt{k} t}{\sqrt{m}}\right] \right\} \right\}$$


$$\left\{ \left\{ y2[t] \rightarrow a + c_1 \cos\left[\frac{\sqrt{k} t}{\sqrt{m}}\right] + c_2 \sin\left[\frac{\sqrt{k} t}{\sqrt{m}}\right] \right\} \right\}$$


$$\{ \{ y3[t] \rightarrow c_1 + t c_2 \} \}$$

```

Relate the qualitative understanding of eigenvectors to the results here.

Eigenvectors corresponds to the fundamental patterns of motion for this 3-mass system,
|特征向量
the normal modes, and the Eigenvalues are the squared frequencies at which each pattern oscillates.
|特征值

Task 4: QSHM:

For the Hermite Polynomials,

```
In[42]:= HermiteH[0, x]  
[埃尔米特多项式]
```

```
HermiteH[1, x]  
[埃尔米特多项式]
```

```
HermiteH[2, x]  
[埃尔米特多项式]
```

```
HermiteH[3, x]  
[埃尔米特多项式]
```

```
Out[42]= 1
```

```
Out[43]= 2 x
```

```
Out[44]= -2 + 4 x2
```

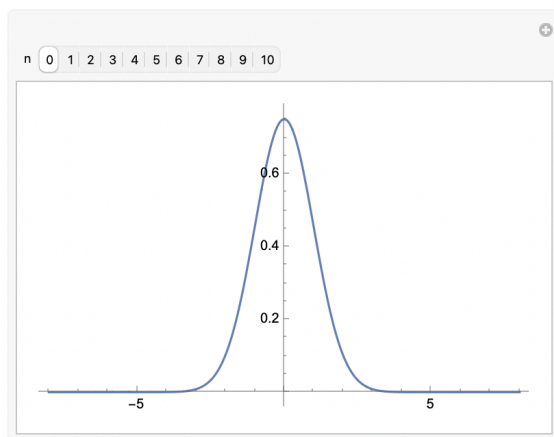
```
Out[45]= -12 x + 8 x3
```

```
In[50]:= Psi[n_] :=  $\frac{1}{\sqrt{2^n \text{Factorial}[n]}} \left(\frac{1}{\pi}\right)^{1/4} e^{-\frac{x^2}{2}}$  HermiteH[n, x]  
[埃尔米特多项式]
```

Let's check this looks sensible

```
In[51]:= Manipulate[  
[交互式操作]  
Plot[Psi[n], {x, -8, 8}, PlotRange -> Full],  
[绘图] [绘制范围] [全范围]  
{n, Range[0, 10],  
[范围]  
ControlType -> Setter}  
[控件类型] [设置按钮]  
]
```

```
Out[51]=
```



Use the above results to construct dH in a smarter way.

Hint: Use nested if statement or a switch statement

If [condition, result_if_true, result_if_false]

Note that the “result_if_false” can be another if statement.

```
In[127]:= dH = Table[Table[
  If[m - n == -4, Coefficient[xhat4psi, psi[n - 4]],
  If[m - n == -2, Coefficient[xhat4psi, psi[n - 2]],
  If[m - n == 0, Coefficient[xhat4psi, psi[n]],
  If[m - n == 2, Coefficient[xhat4psi, psi[n + 2]],
  If[m - n == 4, Coefficient[xhat4psi, psi[n + 4]],
  0
],
],
],
],
{n, 0, 10}],
{m, 0, 10}];
```

```
In[128]:= dH // MatrixForm
|矩阵格式
```

$$\text{Out[128]/MatrixForm=}$$

$$\begin{pmatrix} \frac{3\lambda}{4} & 0 & \frac{3\lambda}{\sqrt{2}} & 0 & \sqrt{\frac{3}{2}}\lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{15\lambda}{4} & 0 & 5\sqrt{\frac{3}{2}}\lambda & 0 & \sqrt{\frac{15}{2}}\lambda & 0 & 0 & 0 & 0 & 0 \\ \frac{3\lambda}{\sqrt{2}} & 0 & \frac{39\lambda}{4} & 0 & 7\sqrt{3}\lambda & 0 & 3\sqrt{\frac{5}{2}}\lambda & 0 & 0 & 0 & 0 \\ 0 & 5\sqrt{\frac{3}{2}}\lambda & 0 & \frac{75\lambda}{4} & 0 & 9\sqrt{5}\lambda & 0 & \sqrt{\frac{105}{2}}\lambda & 0 & 0 & 0 \\ \sqrt{\frac{3}{2}}\lambda & 0 & 7\sqrt{3}\lambda & 0 & \frac{123\lambda}{4} & 0 & 11\sqrt{\frac{15}{2}}\lambda & 0 & \sqrt{105}\lambda & 0 & 0 \\ 0 & \sqrt{\frac{15}{2}}\lambda & 0 & 9\sqrt{5}\lambda & 0 & \frac{183\lambda}{4} & 0 & 13\sqrt{\frac{21}{2}}\lambda & 0 & 3\sqrt{21}\lambda & 0 \\ 0 & 0 & 3\sqrt{\frac{5}{2}}\lambda & 0 & 11\sqrt{\frac{15}{2}}\lambda & 0 & \frac{255\lambda}{4} & 0 & 15\sqrt{14}\lambda & 0 & 3\sqrt{35}\lambda \\ 0 & 0 & 0 & \sqrt{\frac{105}{2}}\lambda & 0 & 13\sqrt{\frac{21}{2}}\lambda & 0 & \frac{339\lambda}{4} & 0 & 51\sqrt{2}\lambda & 0 \\ 0 & 0 & 0 & 0 & \sqrt{105}\lambda & 0 & 15\sqrt{14}\lambda & 0 & \frac{435\lambda}{4} & 0 & 57\sqrt{\frac{5}{2}}\lambda \\ 0 & 0 & 0 & 0 & 0 & 3\sqrt{21}\lambda & 0 & 51\sqrt{2}\lambda & 0 & \frac{543\lambda}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3\sqrt{35}\lambda & 0 & 57\sqrt{\frac{5}{2}}\lambda & 0 & \frac{663\lambda}{4} \end{pmatrix}$$

Verify your method is correct!

```
In[129]:= dH == dHBrute // MatrixForm
|矩阵格式
```

```
Out[129]/MatrixForm=
True
```

The unperturbed harmonic oscillator eigenstates have definite parity: even n give even functions and odd n give odd functions. The x^4 operator (and hence the perturbation dH) is an even function. An even operator only connects states with the same parity, if odd will be zero after integration. In the ground state (which is even), only even-indexed basis states mix in. Thus the coefficients for odd-indexed basis states remain very close to zero.

Now we construct the full matrix. Let's use a smarter way of finding H

```
In[130]:= H = DiagonalMatrix[Table[(n + 1/2), {n, 0, Length[dH] - 1}]] + dH;
```

[对角矩阵] [表格] [长度]

```
H // MatrixForm
```

[矩阵格式]

```
Out[131]//MatrixForm=
```

$$\begin{pmatrix} \frac{1}{2} + \frac{3\lambda}{4} & 0 & \frac{3\lambda}{\sqrt{2}} & 0 & \sqrt{\frac{3}{2}}\lambda & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} + \frac{15\lambda}{4} & 0 & 5\sqrt{\frac{3}{2}}\lambda & 0 & \sqrt{\frac{15}{2}}\lambda & 0 & 0 & 0 & 0 & 0 \\ \frac{3\lambda}{\sqrt{2}} & 0 & \frac{5}{2} + \frac{39\lambda}{4} & 0 & 7\sqrt{3}\lambda & 0 & 3\sqrt{\frac{5}{2}}\lambda & 0 & 0 & 0 & 0 \\ 0 & 5\sqrt{\frac{3}{2}}\lambda & 0 & \frac{7}{2} + \frac{75\lambda}{4} & 0 & 9\sqrt{5}\lambda & 0 & \sqrt{\frac{105}{2}}\lambda & 0 & 0 & 0 \\ \sqrt{\frac{3}{2}}\lambda & 0 & 7\sqrt{3}\lambda & 0 & \frac{9}{2} + \frac{123\lambda}{4} & 0 & 11\sqrt{\frac{15}{2}}\lambda & 0 & \sqrt{105}\lambda & 0 & 0 \\ 0 & \sqrt{\frac{15}{2}}\lambda & 0 & 9\sqrt{5}\lambda & 0 & \frac{11}{2} + \frac{183\lambda}{4} & 0 & 13\sqrt{\frac{21}{2}}\lambda & 0 & 3\sqrt{21}\lambda & 0 \\ 0 & 0 & 3\sqrt{\frac{5}{2}}\lambda & 0 & 11\sqrt{\frac{15}{2}}\lambda & 0 & \frac{13}{2} + \frac{255\lambda}{4} & 0 & 15\sqrt{14}\lambda & 0 & 3\sqrt{35}\lambda \\ 0 & 0 & 0 & \sqrt{\frac{105}{2}}\lambda & 0 & 13\sqrt{\frac{21}{2}}\lambda & 0 & \frac{15}{2} + \frac{339\lambda}{4} & 0 & 51\sqrt{2}\lambda & 0 \\ 0 & 0 & 0 & 0 & \sqrt{105}\lambda & 0 & 15\sqrt{14}\lambda & 0 & \frac{17}{2} + \frac{435\lambda}{4} & 0 & 57\sqrt{\frac{5}{2}}\lambda \\ 0 & 0 & 0 & 0 & 0 & 3\sqrt{21}\lambda & 0 & 51\sqrt{2}\lambda & 0 & \frac{19}{2} + \frac{543\lambda}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3\sqrt{35}\lambda & 0 & 57\sqrt{\frac{5}{2}}\lambda & 0 & \frac{21}{2} + \frac{663\lambda}{4} \end{pmatrix}$$

This Hamiltonian is not diagonal, but will be close to diagonal if λ is small. Let's find the diagonal version of this matrix by numerically finding the eigenvectors. Use Eigensystem[...] and inspect the results

```
In[132]:= physicalValues = {λ → 0.01};
eigsys = Eigensystem[H /. physicalValues] // N;
```

[特征系统] [数值]

```
Print[eigsys[[1]]]
Print[eigsys[[2]][[-1]]]
```

[打印] [打印]

```
{12.4642, 11.0616, 9.40909, 8.21787, 7.04873, 5.90126, 4.77491, 3.6711, 2.59085, 1.53565, 0.507256}
{0.999947, 5.32585 × 10-20, -0.0100028, 1.59208 × 10-18, -0.00257946, 3.56318 × 10-18,
0.000187355, -6.59195 × 10-17, 0.0000179496, 3.74253 × 10-17, -4.24277 × 10-6}
```

Tried it but failed, don't know why...

Use what we have learned in this notebook to make a plot of the groundstate energy as a function of λ .

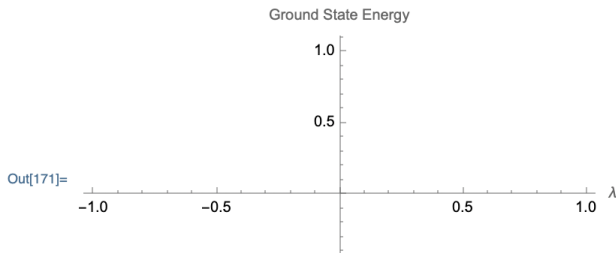
```
In[169]:= groundStateEnergy[lam_] :=
  Min[
    Eigenvalues[N[DiagonalMatrix[Table[n + 1/2, {n, 0, Length[dH] - 1}]] +
      (dH /. {λ → lam})]]] // N

groundStateEnergy[0.01]
Plot[Evaluate[groundStateEnergy[lam]], {lam, 0, 0.1},
  AxesLabel → {"λ", "Ground State Energy"}, PlotRange → All]

... SetDelayed:
(1/4 Root[13366080 + 676602432 λ + 10552490928 λ² + <<5>> + (1953904 + 78727968 λ + 878320872 Power[<<2>>] + 2876920200
  Power[<<2>>] + 1895268375 Power[<<2>>]) #1² + (-163680 - 5211504 λ - 40388040 Power[<<2>>] -
  67151700 Power[<<2>>]) #1³ + <<3>> &, 6])[lam_] 中的标签 Times 被保护.
```

Out[169]= **\$Failed**

```
Out[170]= (1/4 Root[13 366 080 + 676 602 432 λ + 10 552 490 928 λ² + 59 445 761 760 λ³ +
  109 522 759 500 λ⁴ + 45 218 873 700 λ⁵ + 1 404 728 325 λ⁶ + (-9 987 648 - 470 176 608 λ -
  6 582 011 040 λ² - 31 054 106 160 λ³ - 41 229 688 500 λ⁴ - 8 428 369 950 λ⁵) #1 +
  (1 953 904 + 78 727 968 λ + 878 320 872 λ² + 2 876 920 200 λ³ + 1 895 268 375 λ⁴) #1² +
  (-163 680 - 5 211 504 λ - 40 388 040 λ² - 67 151 700 λ³) #1³ +
  (6700 + 148 500 λ + 592 515 λ²) #1⁴ + (-132 - 1518 λ) #1⁵ + #1⁶ &, 6])[0.01]
```



Out[171]=