

## Boas : Ch3 Example 5 p.167

```
Clear["Global`*"]
```

⋮

- **Example 5.** Let's consider a model of a linear triatomic molecule in which we approximate the forces between the atoms by forces due to springs (Figure 12.2).

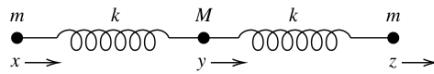


Figure 12.2

### Follow example

```
In[  = pot = + 1/2 k (x - y)^2 + 1/2 k (y - z)^2 // Simplify
```

$$\text{Out}[ = \frac{1}{2} k ((x - y)^2 + (y - z)^2)$$

```
In[  = pot // Expand // Factor
```

$$\text{Out}[ = \frac{1}{2} k (x^2 - 2xy + 2y^2 - 2yz + z^2)$$

```
In[  = {D[pot, x], D[pot, y], D[pot, z]}
```

$$\text{Out}[ = \left\{ k(x - y), \frac{1}{2} k(-2(x - y) + 2(y - z)), -k(y - z) \right\}$$

```
In[  = eqs = -{D[pot, x], D[pot, y], D[pot, z]} == -{m \omega^2 x, M \omega^2 y, m \omega^2 z} // Thread;
eqs // Expand // TableForm
```

*Out[ ]//TableForm=*

$$-kx + ky == -m x \omega^2$$

$$kx - 2ky + kz == -M y \omega^2$$

$$ky - kz == -m z \omega^2$$

```
In[  = eqs = -1/k {D[pot, x], D[pot, y], D[pot, z]} == -1/k {m \omega^2 x, M \omega^2 y, m \omega^2 z} // Thread;
```

*eqs // Expand // TableForm*

*Out[ ]//TableForm=*

$$-x + y == -\frac{m x \omega^2}{k}$$

$$x - 2y + z == -\frac{M y \omega^2}{k}$$

$$y - z == -\frac{m z \omega^2}{k}$$

In[ =]:=  $\text{eqs}[[2]] = \frac{\text{eqs}[[2]]}{M/m}$  // Thread[#, Equal] & // Expand

$$\text{Out}[ = ] = \frac{m x}{M} - \frac{2 m y}{M} + \frac{m z}{M} == -\frac{m y \omega^2}{k}$$

In[ =]:=  $\text{eqs}$  // Expand // TableForm

Out[ = ]//TableForm=

$$\begin{aligned} -x + y &== -\frac{m x \omega^2}{k} \\ \frac{m x}{M} - \frac{2 m y}{M} + \frac{m z}{M} &== -\frac{m y \omega^2}{k} \\ y - z &== -\frac{m z \omega^2}{k} \end{aligned}$$

In[ =]:=  $\text{mat} = \left\{ \{-1, 1, 0\}, \frac{m}{M} \{1, -2, 1\}, \{0, 1, -1\} \right\};$

$\text{mat}$  // MatrixForm

Out[ = ]//MatrixForm=

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

In[ =]:=  $\text{lam} = \lambda \text{DiagonalMatrix}[\{1, 1, 1\}];$

$\text{lam}$  // MatrixForm

Out[ = ]//MatrixForm=

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

In[ =]:=  $\text{mat} - \text{lam}$  // MatrixForm

Out[ = ]//MatrixForm=

$$\begin{pmatrix} -1 - \lambda & 1 & 0 \\ \frac{m}{M} & -\frac{2m}{M} - \lambda & \frac{m}{M} \\ 0 & 1 & -1 - \lambda \end{pmatrix}$$

In[ =]:=  $\text{eq0} = \text{mat} - \text{lam}$  // Det // Factor

$$\text{Out}[ = ] = -\frac{\lambda (1 + \lambda) (2 m + M + M \lambda)}{M}$$

In[ =]:=  $\text{sol} = \text{Solve}[\text{eq0} == 0, \lambda]$  // Simplify

$$\text{Out}[ = ] = \left\{ \{\lambda \rightarrow -1\}, \{\lambda \rightarrow 0\}, \left\{ \lambda \rightarrow -1 - \frac{2m}{M} \right\} \right\}$$

Find Eigenvectors:  $\lambda = \{1, 2, 3\}$

In[ =]:=  $\text{eval} = \text{Eigenvalues}[\text{mat}]$  // Simplify

$$\text{Out}[ = ] = \left\{ 0, -1 - \frac{2m}{M}, -1 \right\}$$

```
In[ 0]:= emat = Eigenvectors [mat]
Out[ 0]= { {1, 1, 1}, {1, -2/M, 1}, {-1, 0, 1} }
```

```
In[ 0]:= sol
Out[ 0]= { {λ → -1}, {λ → 0}, {λ → -1 - 2/M} }
```

## Find first eigenvector

```
In[ 0]:= vec = {x, y, z};
eq1 = mat.vec == λ vec /. sol[[1]] // Thread
Out[ 0]= { -x + y == -x, m x/M - 2 m y/M + m z/M == -y, y - z == -z }
```

```
In[ 0]:= sol1 = Solve[eq1, {x, y, z}]
... Solve : Equations may not give solutions for all "solve" variables.

Out[ 0]= {{y → 0, z → -x}}
```

## Find second eigenvector

```
In[ 0]:= vec = {x, y, z};
eq2 = mat.vec == λ vec /. sol[[2]] // Thread // Simplify
Out[ 0]= { x == y, m (x - 2 y + z)/M == 0, y == z }
```

```
In[ 0]:= sol2 = Solve[eq2[{{1, 2}}], {x, y, z}]
... Solve : Equations may not give solutions for all "solve" variables.

Out[ 0]= {{y → x, z → x}}
```

## Find third eigenvector

```
In[ 0]:= vec = {x, y, z};
eq3 = mat.vec == λ vec /. sol[[3]] // Thread
Out[ 0]= { -x + y == (-1 - 2/M) x, m x/M - 2 m y/M + m z/M == (-1 - 2/M) y, y - z == (-1 - 2/M) z }
```

```
In[ 0]:= Solve[eq3, {x, y, z}]
... Solve : Equations may not give solutions for all "solve" variables.

Out[ 0]= { {y → -2 M x/M, z → x} }
```

## Boas : Ch3 Example 7 p.171

```
In[ = Clear["Global` *"]
```

- **Example 7.** Find the characteristic frequencies and the characteristic modes of vibration for the system of masses and springs shown in Figure 12.3, where the motion is along a vertical line.

### Follow example

```
In[ = tmat = {{4, 0}, {0, 1}};
tmat // MatrixForm
```

Out[ = ]//MatrixForm=

$$\begin{pmatrix} 4 & 0 \\ 0 & 1 \end{pmatrix}$$

```
In[ = vmat = {{4, -1}, {-1, 1}};
vmat // MatrixForm
```

Out[ = ]//MatrixForm=

$$\begin{pmatrix} 4 & -1 \\ -1 & 1 \end{pmatrix}$$

```
In[ = tinv = Inverse[tmat];
tinv // MatrixForm
```

Out[ = ]//MatrixForm=

$$\begin{pmatrix} \frac{1}{4} & 0 \\ 0 & 1 \end{pmatrix}$$

```
In[ = tv = tinv.vmat;
tv // MatrixForm
```

Out[ = ]//MatrixForm=

$$\begin{pmatrix} 1 & -\frac{1}{4} \\ -1 & 1 \end{pmatrix}$$

```
In[ = Eigensystem[tv]
```

```
Out[ = \left\{\left\{\frac{3}{2}, \frac{1}{2}\right\}, \left\{-\frac{1}{2}, 1\right\}, \left\{\frac{1}{2}, 1\right\}\right\}
```

## Change variables

```
In[ = ]:= change = {{1/2, 0}, {0, 1}};
```

```
change // MatrixForm
```

Out[ = ]//MatrixForm=

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

```
In[ = ]:= mat2 = change.vmat.change;
```

```
mat2 // MatrixForm
```

Out[ = ]//MatrixForm=

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

```
In[ = ]:= Eigensystem[mat2]
```

$$\left\{ \left\{ \frac{3}{2}, \frac{1}{2} \right\}, \left\{ \{-1, 1\}, \{1, 1\} \right\} \right\}$$

```
In[ = ]:= evecs = Normalize /@ Eigenvectors[mat2]
```

$$\left\{ \left\{ -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right\}, \left\{ \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right\} \right\}$$

```
In[ = ]:= Transpose[evecs].evecs // MatrixForm
```

Out[ = ]//MatrixForm=

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