

$$\hat{H} = \hat{T} + \hat{V}$$

$$\{\phi_i\} = \{\phi_1, \phi_2, \phi_3, \dots\}$$

$$\mathbf{H} = \langle i | \hat{H} | j \rangle$$

$$\hat{H} | j \rangle = \sum_k h_k^{(j)} | k \rangle$$

$$\langle i | \hat{H} | j \rangle = \sum_k h_k^{(j)} \langle i | k \rangle$$

$$\hat{H} \psi_n = E_n \psi_n$$

$$\mathbf{H} = \begin{pmatrix} \langle 0 | \hat{H} | 0 \rangle & \langle 0 | \hat{H} | 1 \rangle & \square & & \square \\ \langle 1 | \hat{H} | 0 \rangle & & \dots & \square & \square \\ & \dots & & \square & \square \\ & & \square & \square & \square \\ & \square & & \square & \square \end{pmatrix} \begin{matrix} \langle 0 | \hat{H} | 0 \rangle \\ \langle 0 | \hat{H} | 1 \rangle \\ \dots \\ \langle N | \hat{H} | N \rangle \end{matrix}$$

$$\mathbf{H}\Psi = \mathbf{E}\Psi$$

$$\mathbf{H}\psi_0 = E_0\psi_0$$

$$\mathbf{H}\psi_1 = E_1\psi_1$$

$$\dots$$

$$\mathbf{H}\psi_N = E_N\psi_N$$

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a = RandomReal[{}], {100, 100}];
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H = a + Transpose[a];
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{engs, wfns} = Eigensystem[H];
```

$$\psi_n = \sum_k c_k^{(n)} | k \rangle$$

```
In[122]:= engs
```

```
Out[122]= {101.179, -8.0043, 7.92349, 7.59313, -7.58848, 7.32018, -7.06523, 7.00818,
6.76508, -6.65089, 6.43429, -6.4266, 6.39575, 6.27105, -6.10927, 6.10148,
-6.09574, 5.93028, -5.92146, -5.72323, 5.70458, 5.61429, -5.49158,
5.3708, -5.28453, -5.24087, 5.18209, -5.08459, 5.05129, -4.97488, 4.91607,
4.81369, -4.67693, 4.64648, -4.4636, -4.36362, 4.35003, -4.28172, 4.22549,
4.12278, -4.03745, 3.88197, -3.87642, 3.83535, -3.74428, -3.65675, 3.58449,
-3.58195, 3.37729, 3.3429, -3.24621, 3.22717, -3.20706, 3.10843, -3.0553,
-2.98217, 2.92626, -2.88503, 2.79667, -2.70177, 2.67188, -2.50373, 2.4846,
-2.47168, -2.33024, -2.27519, 2.24029, 2.08236, 1.9281, -1.86432, -1.81028,
1.78309, 1.70112, -1.63967, 1.61751, -1.50347, 1.42892, -1.41947, 1.32968,
-1.25449, 1.16168, 1.09375, -1.05284, 0.88105, -0.880825, -0.753754,
0.73197, -0.724547, 0.578093, -0.567645, 0.50635, 0.499356, 0.428357,
-0.40143, -0.272378, 0.26503, -0.172787, -0.131066, -0.117469, 0.020895}
```

```
In[123]:= wfns // Dimensions
```

```
Out[123]= {100, 100}
```

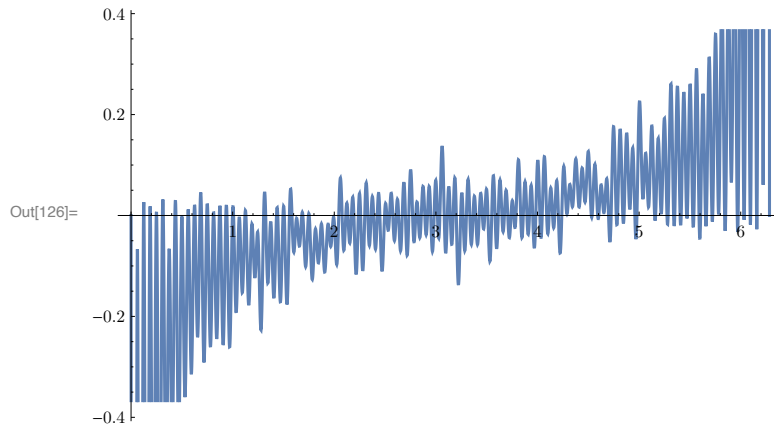
In[124]:= wfns[[1]]

Out[124]= {-0.104087, -0.102147, -0.0904153, -0.0982184, -0.0967095, -0.102407, -0.10094,  
-0.104582, -0.0963196, -0.100479, -0.101242, -0.0949961, -0.0913744,  
-0.104545, -0.103744, -0.101432, -0.101754, -0.107876, -0.0973557, -0.100665,  
-0.102276, -0.103714, -0.100987, -0.100313, -0.096739, -0.109312, -0.103588,  
-0.100071, -0.101338, -0.0982598, -0.0994516, -0.100375, -0.0965511,  
-0.103241, -0.0999661, -0.104298, -0.101629, -0.0996022, -0.102558,  
-0.0991022, -0.104669, -0.0997378, -0.101963, -0.0968098, -0.102322,  
-0.101642, -0.102079, -0.0935485, -0.0976752, -0.0989465, -0.106983,  
-0.0971894, -0.0985047, -0.106615, -0.105776, -0.105726, -0.102562,  
-0.0935267, -0.0986888, -0.0988274, -0.100832, -0.0901811, -0.0966173,  
-0.0943959, -0.0954381, -0.102123, -0.100358, -0.0883129, -0.0973674,  
-0.103334, -0.101425, -0.104078, -0.0973132, -0.101117, -0.104361, -0.0922964,  
-0.0955305, -0.0976166, -0.103185, -0.0946714, -0.0986926, -0.100092,  
-0.0976793, -0.0997751, -0.0985439, -0.108618, -0.0972537, -0.0966342,  
-0.0964978, -0.102026, -0.106624, -0.104135, -0.0925356, -0.102311,  
-0.0978287, -0.0945822, -0.0963842, -0.107477, -0.0950313, -0.0995666}

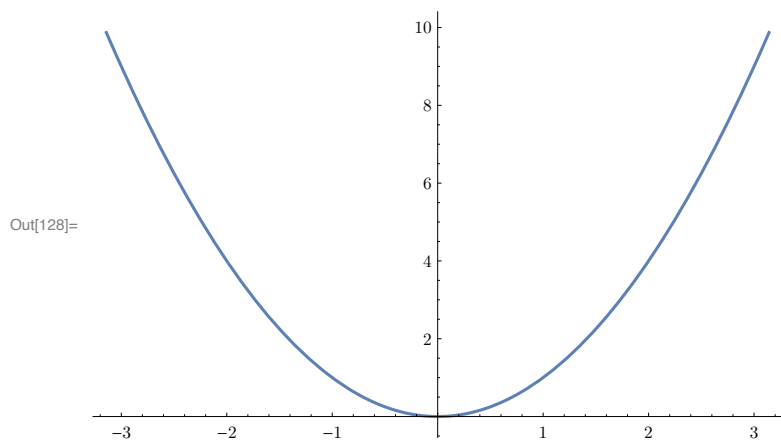
$$H \Psi = E \Psi$$

$$\psi_n = \sum_i c_i^{(n)} \phi_i$$

In[126]:= Plot[Sum[wfns[[1, i]] \* Sin[i \* x], {i, 100}], {x, 0, 2 π}]



In[128]:= **Plot**[x^2, {x, -π, π}]



In[134]:= **potRep**[i\_, j\_] := **Integrate**[**Sin**[i \* x] \* x^2 \* **Sin**[j \* x], {-π, π}]

**potRep**[

In[132]:= **keRep**[i\_, j\_] := **Integrate**[**Sin**[i \* x] \* **D**[**Sin**[j \* x], {x, 2}], {x, -π, π}]

In[133]:= **keRep**[i, j]

Out[133]= 
$$\frac{2 j^2 (j \cos[j \pi] \sin[i \pi] - i \cos[i \pi] \sin[j \pi])}{-i^2 + j^2}$$

In[129]:= **D**[**Sin**[j \* x], {x, 2}]

Out[129]=  $-j^2 \sin[j x]$