Calculate energies of three lowest states of the He atom using 3 basis states (energies are in atomic unit)

Note: we show the codes for the calculations using 3 basis states here so that the result can be directly compared to our analytic calculation in our research article. Line 2 of the code can then be changed to various number of basis states. In our article, we vary the number of basis states from n = 3 to n = 25.

Define radial wave function, i.e. the equation (16) in the research article.

```
Pn_[r_] := Sqrt[(2 (n - 1)!)/(n^2 (n)!)] (4 r/n) e^(-2 r/n) LaguerreL[n - 1, 1, 4 r/n]
```

Generate the list of states. Here, we use 3 basis states as shown in equation (19) in the article. This can be changed to various number of basis states.

```
st = DeleteDuplicates[Table[{{1, i}, {i, 1}}, {i, 2}] ~Flatten~ 1]
```

```
{{1, 1}, {1, 2}, {2, 1}}
```

Calculate unperturbed energy of the He+ ion, i.e. equation (11) in the text

```
E0[{n1_, n2_}] := -2/n1^2 + -2/n2^2
```

Evaluate the matrix elements of the potential, i.e. the second term of the equation (14) in the text.

```
V[{n1_, n2_}, {n3_, n4_}] :=
  NIntegrate[
   Pn1[r1] Pn3[r1] Min[1/r2, 1/r1] Pn2[r2] Pn4[r2], {r2, 0, ∞}, {r1, 0, ∞}];
```

Calculate all the elements of the Hamiltonian matrix, i.e. equation (14) in the text

```
H = DiagonalMatrix[E0 /@ st] +
    Table[V[st[[i]], st[[j]]], {i, Length[st]}, {j, Length[st]}];
```

Show the Hamiltonian matrix which can be compared to analytic calculations in equation (29) in the text

```
H // MatrixForm
```

$$\begin{pmatrix} -2.75 & 0.17871 & 0.17871 \\ 0.17871 & -2.08025 & 0.0438957 \\ 0.17871 & 0.0438957 & -2.08025 \end{pmatrix}$$

Calculate and show the eigenvalues for 1s1s, 1s2s triplet, and 1s2s singlet; the results are then compared to the analytic caculations shown in equation (30) in the text

```
eval = Eigenvalues[H][[ ;; 3]]; eval
```

```
{-2.83044, -2.12414, -1.95591}
```