

Solutions for l-states of Diatomic Molecules under the Modified-Morse Potential using the Nikiforov-Uvarov Functional Analysis (NUFA) Method

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```
In[1]:= (*Define subscripted symbols*)
Notation`AutoLoadNotationPalette = False;
<< Notation`;
Symbolize /@
{ $\alpha_1$ ,  $\alpha_2$ ,  $\alpha_3$ ,  $\xi_1$ ,  $\xi_2$ ,  $\xi_3$ ,  $E_{nl}$ ,  $\psi_{nl}$ ,  $D_e$ ,  $r_e$ ,  $V_{rot}$ ,  $X_1$ ,  $X_2$ ,  $X_3$ };
```

Part 2: NUFA Calculations

We use the parameters and energy equation found in Part-1: Algebra to solve for numerical values of energy eigenvalues and corresponding eigenfunctions.

```
In[4]:= (*Importing Dataset of Spectroscopic Constants*)
molecularData = Import[
  "G:\\My Drive\\Research Projects\\Computational Quantum Mechanics\\Nikiforov-Uvarov
  Method\\molecular_data.csv", {"CSV", "Dataset"}, "HeaderLines" -> {1, 1}]
```

	D_e	r_e	mu	alpha
H2	4.7446	0.7416	0.50391	1.44056
LiH	2.51529	1.5956	0.880122	1.79984
HCl	4.61907	1.2746	0.980104	2.38057
CO	11.2256	1.1283	6.86067	2.59441

Molecular Parameters

```
In[5]:= molecule = "CO";
{D_e, r_e,  $\mu$ ,  $\alpha$ } = {"D_e", "r_e", "mu", "alpha"} /. Normal[molecularData[molecule]];
(*amu to eV/c2*)
 $\mu$  =  $\mu * 931.494 * 10^6$ ;
 $\hbar$  = 1973;
```

NUFA Parameters

All assignments below are delayed. They are evaluated afresh each time they are called, so that we get correct values if we change the molecular parameters and quantum numbers.

```

In[9]:=  $\beta := \frac{2 \mu r_e^2}{\alpha^2 \hbar^2};$ 

 $X_1 := D_e + \frac{\hbar^2 \ell (\ell + 1)}{2 \mu r_e^2} \left( \frac{3}{\alpha^2} - \frac{1}{\alpha} \right);$ 

 $X_2 := -2 D_e + \frac{\hbar^2 \ell (\ell + 1)}{2 \mu r_e^2} \left( -\frac{6}{\alpha^2} + \frac{4}{\alpha} \right);$ 

 $X_3 := \frac{\hbar^2 \ell (\ell + 1)}{2 \mu r_e^2} \left( 1 + \frac{3}{\alpha^2} - \frac{3}{\alpha} \right);$ 

 $\lambda := \sqrt{\beta X_1};$ 

 $\nu := \sqrt{\beta (-E_{n\ell} + X_3)};$ 

```

Energy Eigenvalues

Define the quantum numbers n and ℓ and call the expression below to get the eigenvalue.

```

In[15]:=  $E_{n\ell} := \left( X_3 - \frac{1}{\beta} \left( \frac{1}{2} + n + \frac{X_2}{2} \sqrt{\frac{\beta}{X_1}} \right)^2 \right);$ 

```

```

In[16]:= (*Example*)
n = 1;
l = 5;
StringForm[
  "Energy Eigenvalue for `` under the Modified-Morse Potential; n = ``, l = ``: `` eV",
  molecule, n, l, NumberForm[En $\ell$ , 10]]

```

```

Out[18]=
Energy Eigenvalue for CO under the
Modified-Morse Potential; n = 1, l = 5: -10.8187914 eV

```

Eigenfunctions

We use the expression for eigenfunctions given in Udoh et al. Their numerical values are too small to be plotted accurately, so we numerically integrate and normalize them. We also need to reverse the change of variables made in Part-1, i.e., $z = e^{\frac{-\alpha(r-r_e)}{r_e}}$ because we will be plotting the eigenfunctions along the r -axis.

```

In[19]:= (*Non-Normalized Eigenfunction*)
nonNormalizedEigenfunction[r_] :=
  FullSimplify[ (e-λ z zν Hypergeometric1F1[-n, (1 + 2 ν), 2 λ z]) /. {z → e-α  $\frac{(r-r_e)}{r_e}$ } ];
(*Normalization Constant*)
N := NIntegrate[(nonNormalizedEigenfunction[r])2, {r, 0, ∞}];
(*Normalized Eigenfunction*)
ψn $\ell$ [r_] := FullSimplify[  $\frac{1}{\sqrt{N}}$  nonNormalizedEigenfunction[r] ];

```

Tabulating and Plotting

```
In[22]:= (*Eigenvalues*)
nMin = 0;
nMax = 10;
lMin = 0;
lMax = 5;
Labeled[
  Grid[Table[NumberForm[Enl, {20, 7}], {n, nMin, nMax}, {l, lMin, lMax}], Frame → All],
  StringForm["Energy Eigenvalues (eV) for `` under the Modified-Morse Potential",
    molecule], Top]
(*n on rows, l on columns*)
```

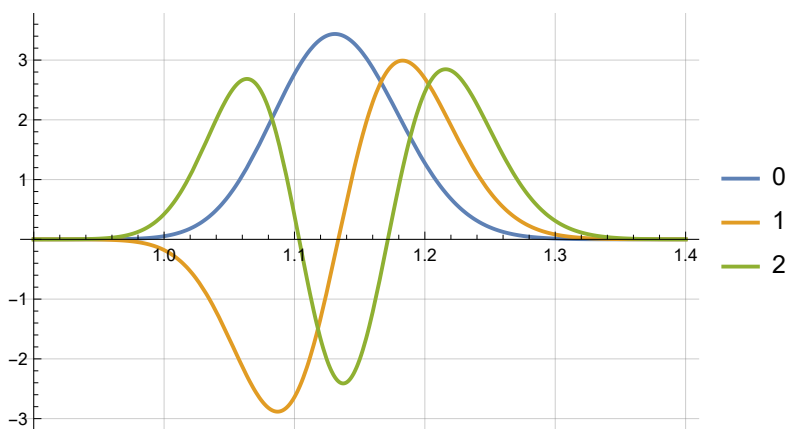
Out[26]=

Energy Eigenvalues (eV) for CO under the Modified-Morse Potential

-11.0915536	-11.0910772	-11.0901243	-11.0886951	-11.0867895	-11.0844077
-10.8258762	-10.8254038	-10.8244591	-10.8230421	-10.8211529	-10.8187914
-10.5634194	-10.5629511	-10.5620146	-10.5606098	-10.5587368	-10.5563957
-10.3041832	-10.3037190	-10.3027906	-10.3013980	-10.2995413	-10.2972206
-10.0481676	-10.0477075	-10.0467872	-10.0454068	-10.0435664	-10.0412660
-9.7953726	-9.7949165	-9.7940044	-9.7926362	-9.7908121	-9.7885321
-9.5457981	-9.5453461	-9.5444422	-9.5430862	-9.5412784	-9.5390188
-9.2994443	-9.2989964	-9.2981005	-9.2967568	-9.2949653	-9.2927260
-9.0563111	-9.0558672	-9.0549795	-9.0536480	-9.0518728	-9.0496538
-8.8163984	-8.8159586	-8.8150791	-8.8137598	-8.8120008	-8.8098023
-8.5797063	-8.5792706	-8.5783992	-8.5770921	-8.5753495	-8.5731713

```
In[27]:= (*Eigenfunctions*)
Plot[Evaluate[Table[ψnl[r]], {n, 0, 2}]], {r, 0.9, 1.4},
  PlotRange → Automatic, PlotLegends → Range[0, 2], GridLines → Automatic]
```

Out[27]=



```
In[28]:= (*Probability Densities*)
```

```
Plot[Evaluate[Table[( $\psi_n[r]$ )2, {n, 0, 2}]], {r, 0.9, 1.4},  
PlotRange → Automatic, PlotLegends → Range[0, 2], GridLines → Automatic]
```

Out[28]=

