Taller de Química Cuántica.

Material para el curso de Fisicoquímica IV .

1. Los fundamentos de la mecánica cuántica.

1.A. Los antecedentes de la teoría cuántica.

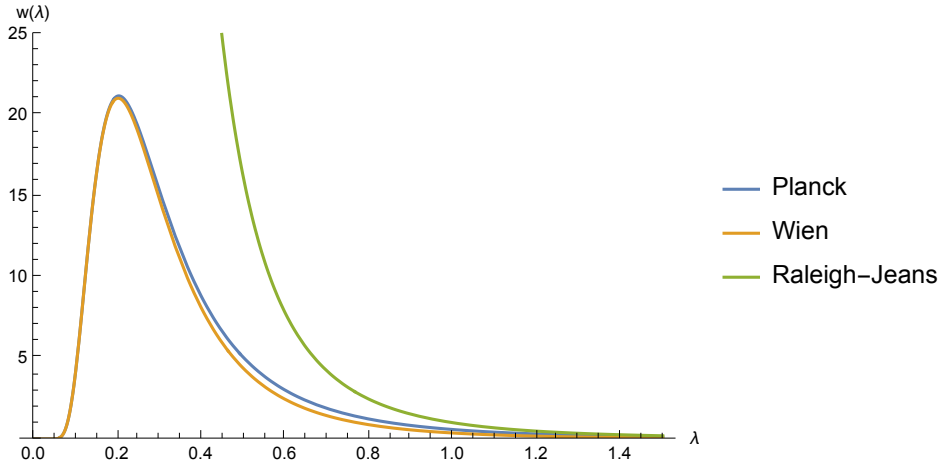
1.A.1. La radiación del cuerpo negro.

Las distribuciones.

Las gráficas.

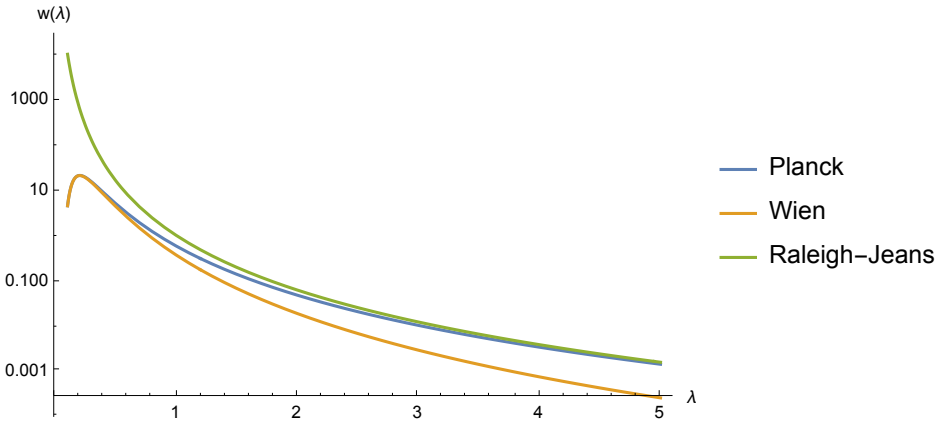
In[•]:=
```
Plot[{wp[1, x], ww[1, x], wrj[1, x]}, {x, 0, 1.5}, PlotRange → {0, 25},
 AxesLabel → {"λ", "w(λ)"}, PlotLegends → {"Planck", "Wien", "Raleigh-Jeans"}]
```

Out[•]=



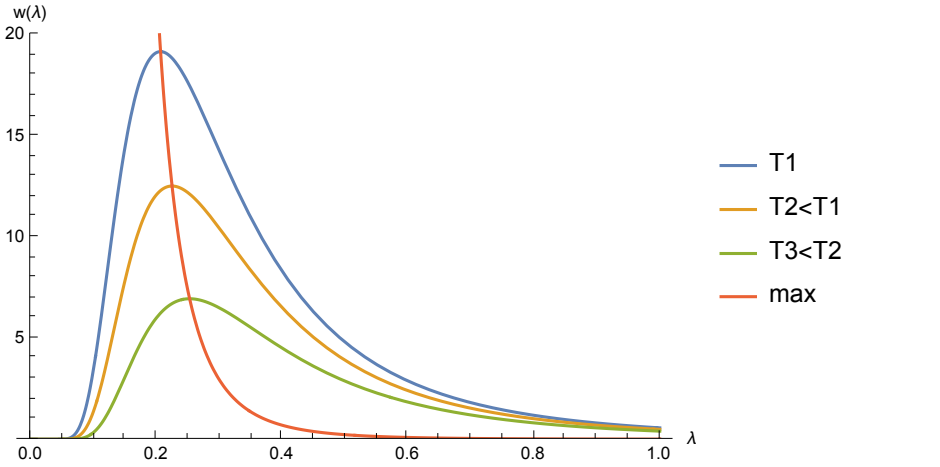
In[•]:=
```
LogPlot[{wp[1, x], ww[1, x], wrj[1, x]}, {x, 0.1, 5},
 AxesLabel → {"λ", "w(λ)"}, PlotLegends → {"Planck", "Wien", "Raleigh-Jeans"}]
```

Out[•]=



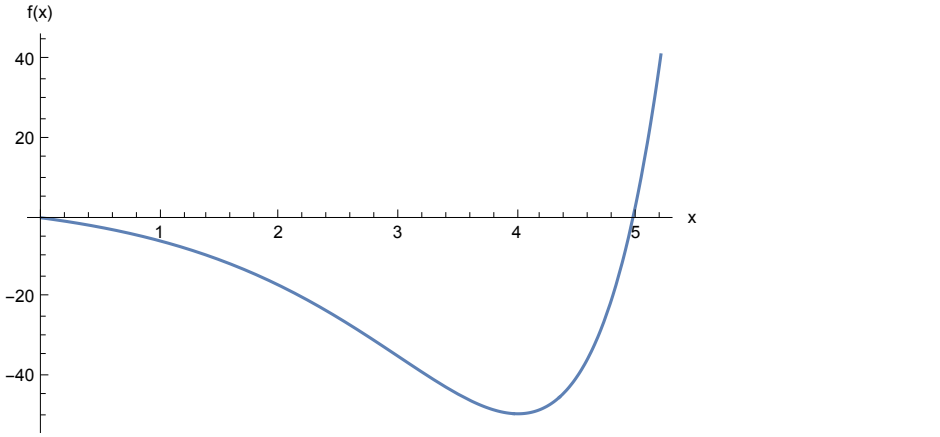
In[•]:=
```
Plot[{wp[0.98, x], wp[0.90, x], wp[0.80, x], 1 / (x^5 * (Exp[4.965] - 1))},
 {x, 0, 1}, PlotRange → {0, 20}, AxesLabel → {"λ", "w(λ)"},
 PlotLegends → {"T1", "T2<T1", "T3<T2", "max"}]
```

Out[•]=



In[•]:=
```
Plot[Exp[x] * (x - 5) + 5, {x, 0, 5.2}, AxesLabel → {"x", "f(x)"}]
```

Out[•]=



1.B. Los principios de la teoría cuántica.

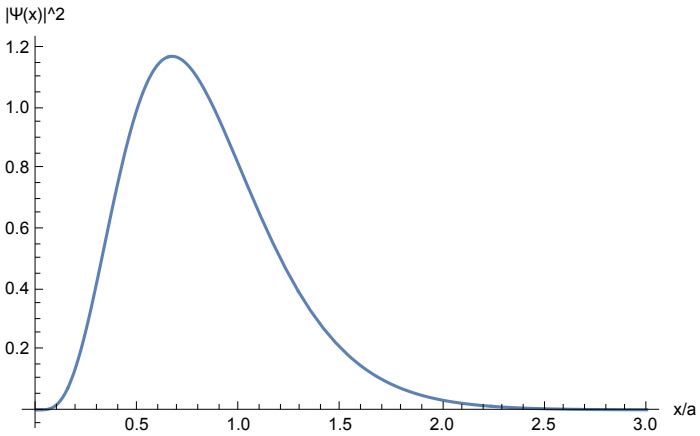
1.B.1. Las funciones de onda.

In[•]:=
```
fonda1[x_] := 18 * x^2 * Exp[-3 * x];
```

In[•]:=
```
Print[TraditionalForm[fonda1[x]^2]]
Plot[fonda1[x]^2, {x, 0, 3}, AxesLabel → {"x/a", "|Ψ(x)|^2"}]
```

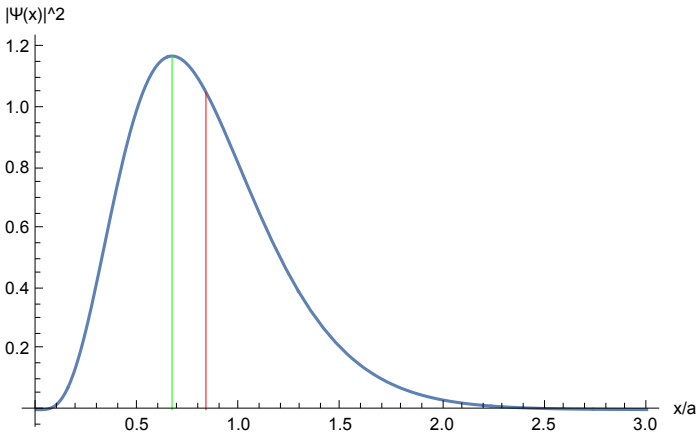
$324\, e^{-6x}\, x^4$

Out[•]=



In[•]:=
```
Show[Plot[fonda1[x]^2, {x, 0, 3}, AxesLabel → {"x/a", "|Ψ(x)|^2"}],
 Graphics[{Green, Line[{{2 / 3, fonda1[2 / 3]^2}, {2 / 3, 0}}]}],
 Graphics[{Red, Line[{{5 / 6, fonda1[5 / 6]^2}, {5 / 6, 0}}]}]]
```

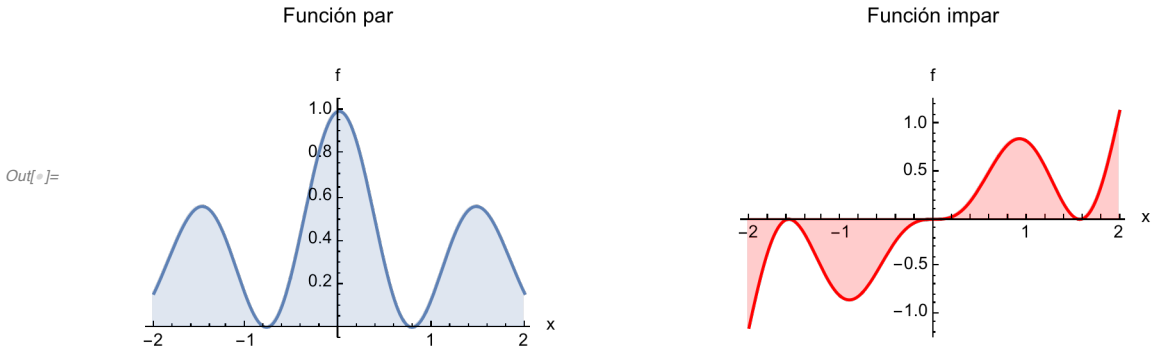
Out[•]=



La paridad de las funciones y el área bajo la curva.

In[•]:=
```
GraphicsGrid[{{Plot[Cos[2 * x] ^ 2 * Exp[-x ^ 2 / 4], {x, -2, 2},
    Filling → Axis, PlotLabel → "Función par", AxesLabel → {"x", "f"}],
  Plot[Sin[2 * x] ^ 2 * x, {x, -2, 2}, Filling → Axis, PlotStyle → Red,
   PlotLabel → "Función impar", AxesLabel → {"x", "f"}]}}]
```

Out[•]=



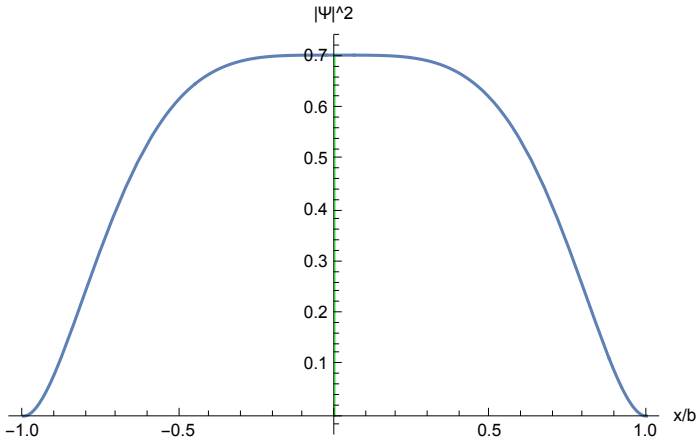
Otras densidades de probablilidad.

In[•]:=
```
fonda2[x_] := Sqrt[45] / 8 * (1 - x ^ 4);
fonda3[x_] := Sqrt[105] * x ^ 2 * (1 - x);
```

In[•]:=
```
Print[TraditionalForm[fonda2[x] ^ 2]]
Show[Plot[fonda2[x] ^ 2, {x, -1, 1}, AxesLabel → {"x/b", "|Ψ|^2"}],
 Graphics[{Green, Line[{{0, 0}, {0, fonda2[0] ^ 2}}]}],
 Graphics[{Red, Line[{{0, 0}, {0, fonda2[] 0} ^ 2}]}]]
```

$$\frac{45}{64}\left(1 - x^4\right)^2$$

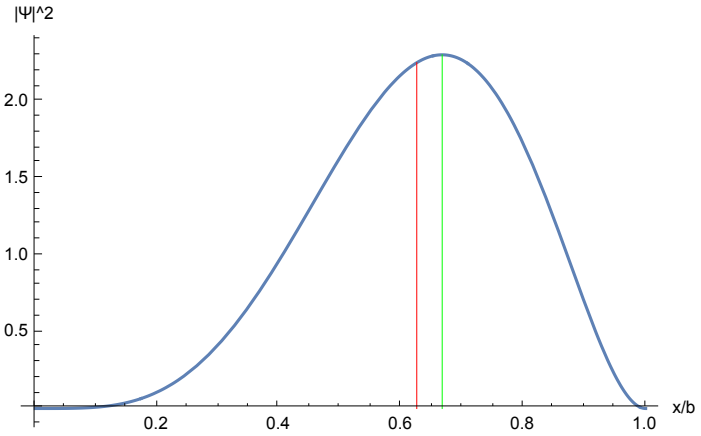
Out[•]=



In[•]:=
```
Print[TraditionalForm[fonda3[x]^2]]
Show[Plot[fonda3[x]^2, {x, 0, 1}, AxesLabel → {"x/b", "|Ψ|^2"}],
 Graphics[{Green, Line[{{2 / 3, 0}, {2 / 3, fonda3[2 / 3]^2}}]}],
 Graphics[{Red, Line[{{5 / 8, 0}, {5 / 8, fonda3[5 / 8]^2}}]}]]
```

$$105\ (1-x)^2\ x^4$$

Out[•]=



2. Algunos sistemas sencillos.

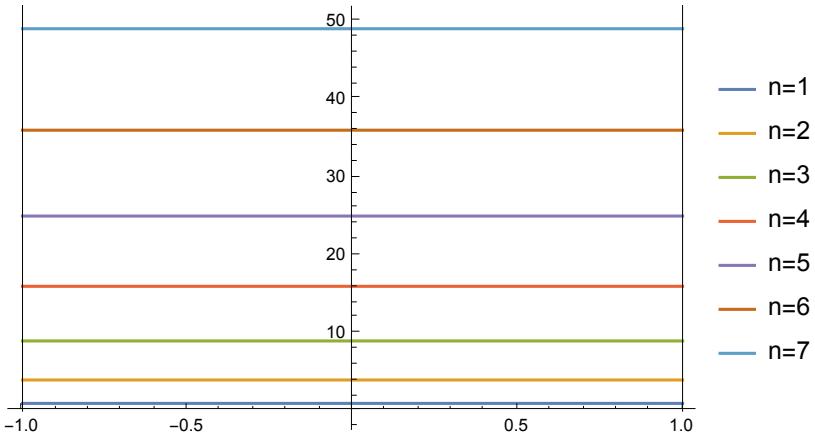
2.A. El movimiento traslacional.

2.A.1. La partícula encerrada entre [-a,a].

El espectro.

In[•]:=
```
Show[Plot[{1, 4, 9, 16, 25, 36, 49}, {x, -1, 1},
  PlotLegends → {"n=1", "n=2", "n=3", "n=4", "n=5", "n=6", "n=7"}],
 Graphics[{Black, Line[{{-1, 0}, {-1, 52}}]}],
 Graphics[{Black, Line[{{1, 0}, {1, 52}}]}]]
```

Out[•]=

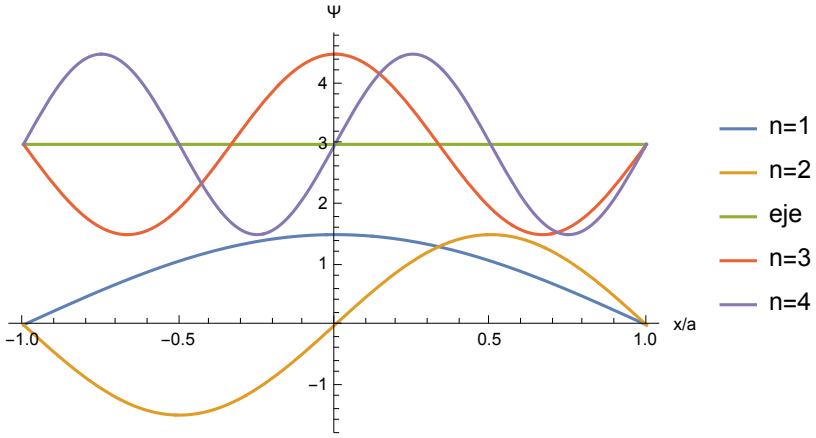


Las funciones de onda.

In[•]:=
```
trfop[x_, n_, a_] := a * Cos[n * x * Pi / 2];
trfoi[x_, n_, a_] := a * Sin[n * x * Pi / 2];
```

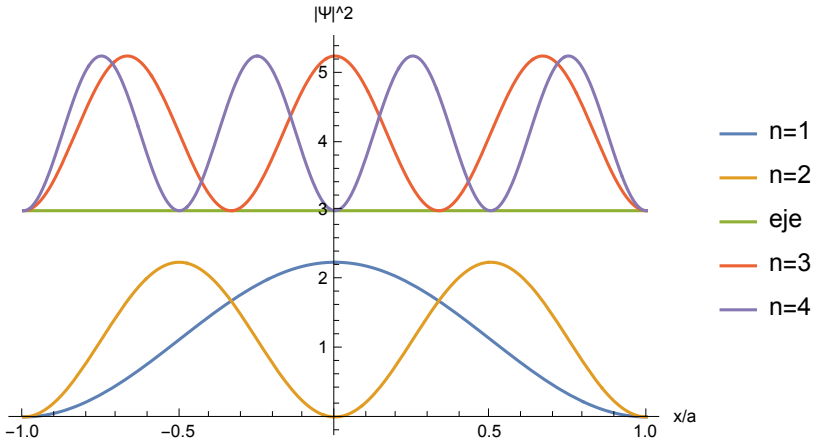
In[•]:=
```
Plot[{trfop[x, 1, 1.5], trfoi[x, 2, 1.5],
  3, trfop[x, 3, 1.5] + 3, trfoi[x, 4, 1.5] + 3}, {x, -1, 1},
 AxesLabel → {"x/a", "Ψ"}, PlotLegends → {"n=1", "n=2", "eje", "n=3", "n=4"}]
```

Out[•]=



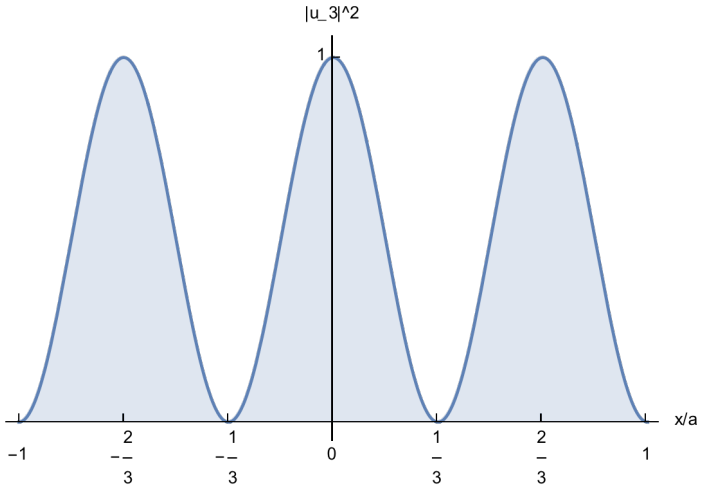
In[•]:=
```
Plot[{trfop[x, 1, 1.5]^2, trfoi[x, 2, 1.5]^2, 3,
  trfop[x, 3, 1.5]^2 + 3, trfoi[x, 4, 1.5]^2 + 3}, {x, -1, 1},
 AxesLabel → {"x/a", "|Ψ|^2"}, PlotLegends → {"n=1", "n=2", "eje", "n=3", "n=4"}]
```

Out[•]=



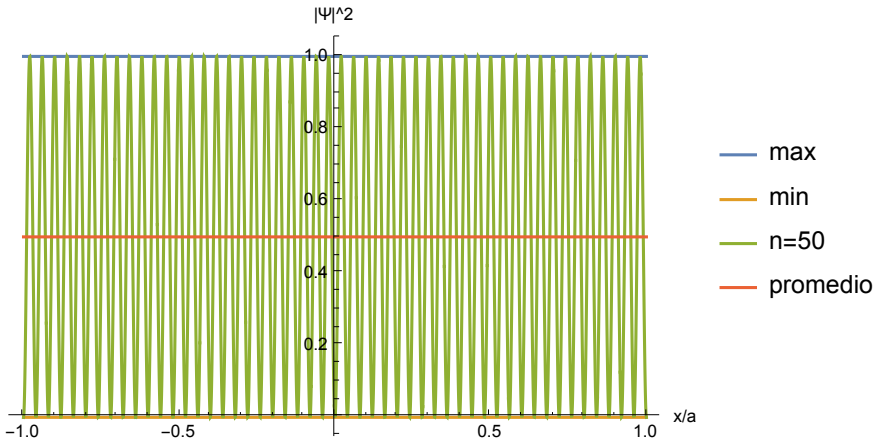
In[•]:=
```
Plot[trfop[x, 3, 1]^2, {x, -1, 1}, AxesLabel → {"x/a", "|u_3|^2"},
 Filling → Axis, Ticks → {{-1, -2/3, -1/3, 0, 1/3, 2/3, 1}, {0, 1}}]
```

Out[•]=



In[•]:=
```
Plot[{1, 0, trfoi[x, 50, 1]^2, 0.5}, {x, -1, 1},
 AxesLabel → {"x/a", "|Ψ|^2"}, PlotLegends → {"max", "min", "n=50", "promedio"}]
```

Out[•]=



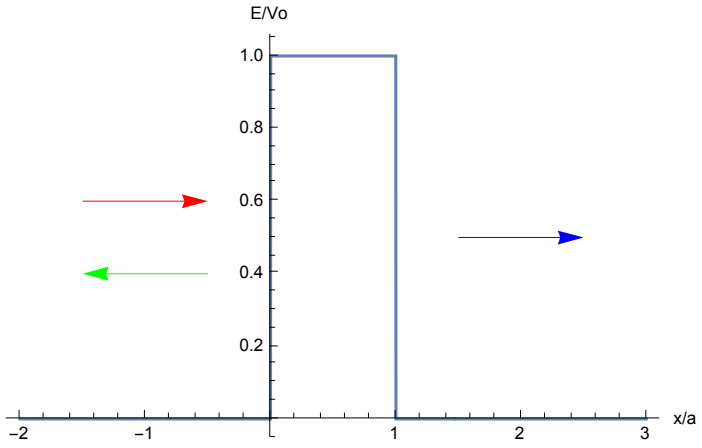
2.A.2. La barrera de potencial.

La funciones

La energía potencial.

In[•]:=
```
Show[Plot[If[e > 0 && e < 1, 1, 0], {e, -2, 3}, AxesLabel → {"x/a", "E/Vo"}],
 Graphics[{Blue, Arrow[{{1.5, 0.5}, {2.5, 0.5}}]}],
 Graphics[{Red, Arrow[{{-1.5, 0.6}, {-0.5, 0.6}}]}],
 Graphics[{Green, Arrow[{{-0.5, 0.4}, {-1.5, 0.4}}]}]]
```

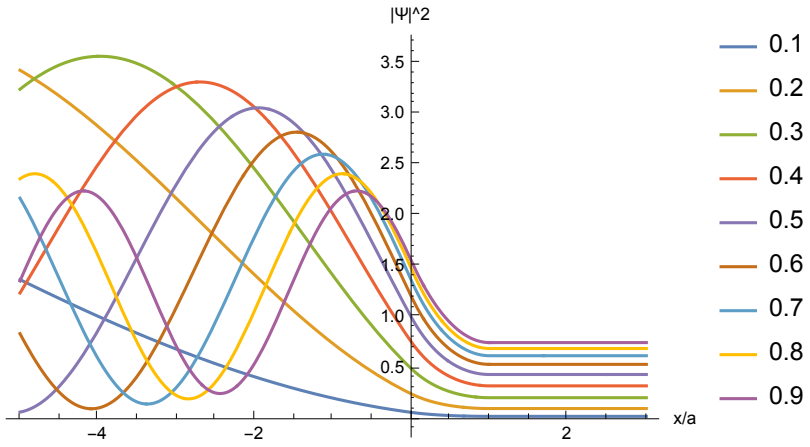
Out[•]=



Las densidades de probabilidad para E < Vo.

In[•]:=
```
Plot[Evaluate[Table[P[x, 1, 0.1 * i], {i, 9}]], {x, -5, 3},
 PlotLegends → Table[0.1 * i, {i, 9}], AxesLabel → {"x/a", "|Ψ|^2"}]
```

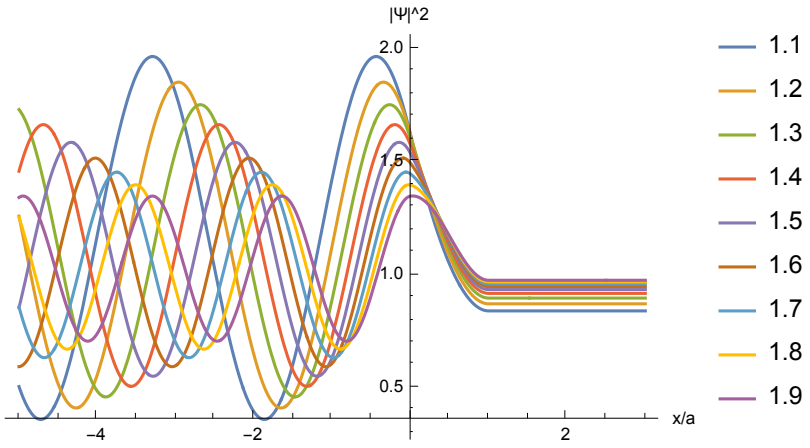
Out[•]=



Las densidades de probabilidad para E > Vo.

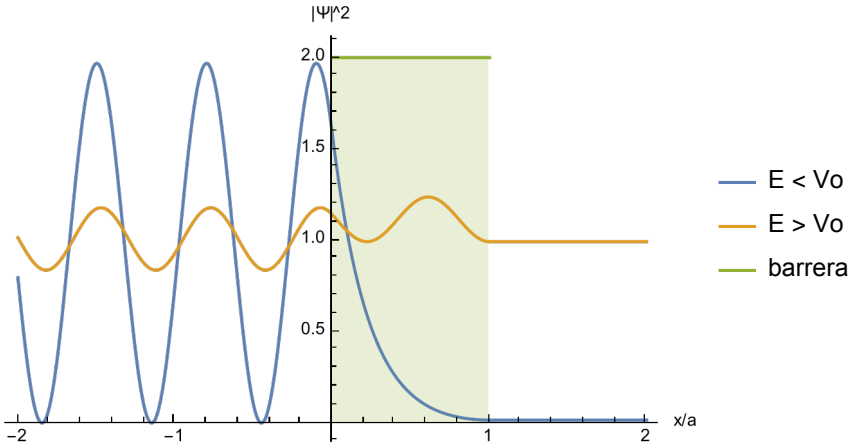
In[•]:=
```
Plot[Evaluate[Table[P1[x, 1, 1 + 0.1 * i], {i, 9}]], {x, -5, 3},
 PlotLegends → Table[1 + 0.1 * i, {i, 9}], AxesLabel → {"x/a", "|Ψ|^2"}]
```

Out[•]=



In[•]:=
```
Plot[{P[x, 5, 4.5] / 2, P1[x, 2, 4.5], If[x > 0 && x < 1, 2]},
 {x, -2, 2}, AxesLabel → {"x/a", "|Ψ|^2"},
 PlotLegends → {"E < Vo", "E > Vo", "barrera"}, Filling → {3 → Bottom}]
```

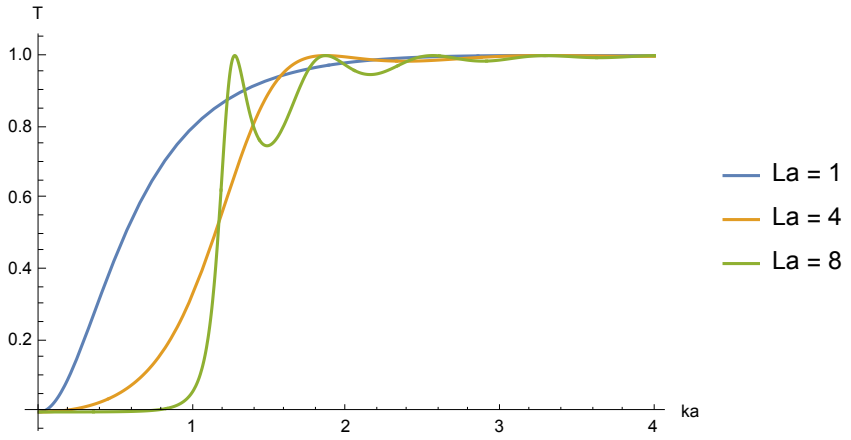
Out[•]=



La transmisión a través de una barrera.

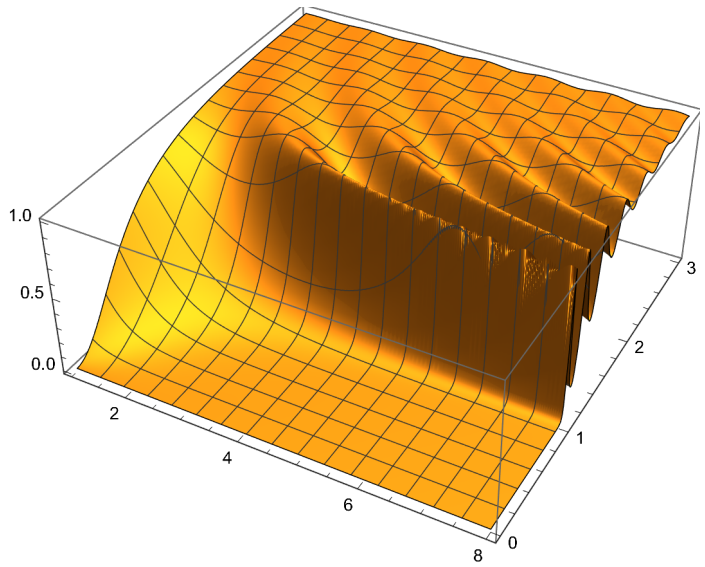
In[•]:=
```
Plot[{tbar[k, 1], tbar[k, 2], tbar[k, 4]}, {k, 0, 4},
 AxesLabel → {"ka", "T"}, PlotLegends → {"La = 1", "La = 4", "La = 8"}]
```

Out[•]=



In[•]:=
```
Plot3D[tbar[k, l], {l, 1, 8}, {k, 0, 3}, PlotPoints → 100]
```

Out[•]=



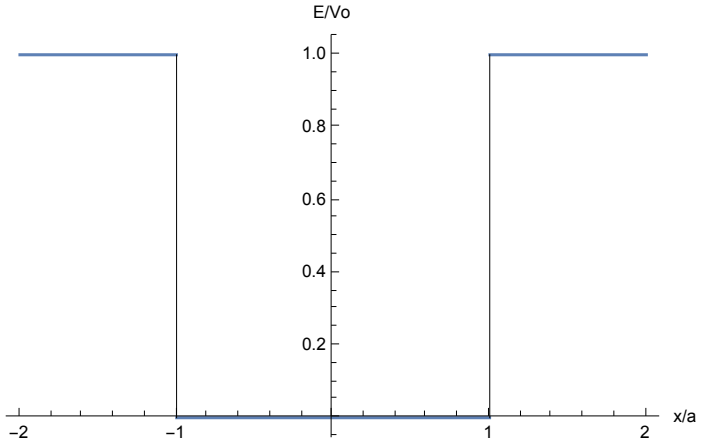
2.A.3. El pozo finito de potencial.

Las funciones.

La energía potencial.

In[•]:=
```
Show[Plot[If[Abs[e] < 1, 0, 1], {e, -2, 2}, AxesLabel → {"x/a", "E/Vo"}],
 Graphics[{Black, Line[{{-1, 0}, {-1, 1}}]}],
 Graphics[{Black, Line[{{1, 0}, {1, 1}}]}]]
```

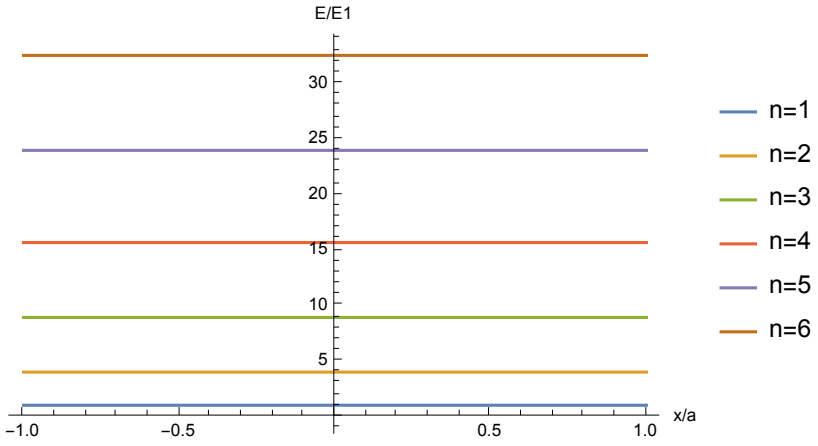
Out[•]=



El espectro y las funciones propias para E < Vo.

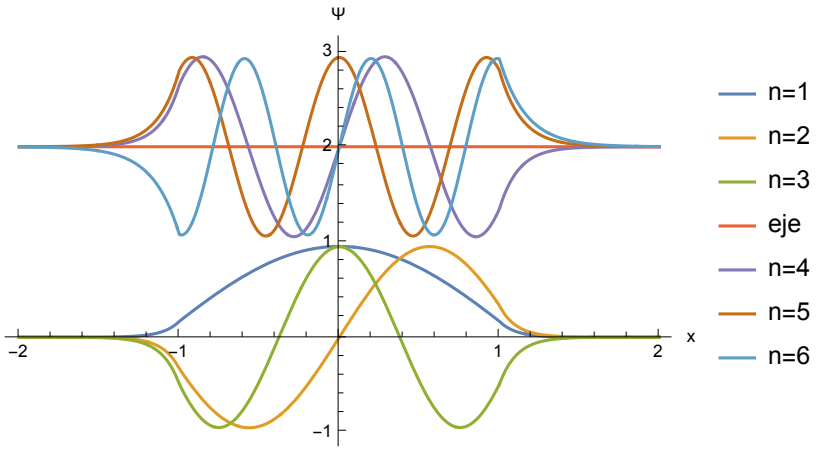
```
Plot[epozo, {x, -1, 1}, AxesLabel → {"x/a", "E/E1"},
 PlotLegends → {"n=1", "n=2", "n=3", "n=4", "n=5", "n=6"}]
```

Out[•]=



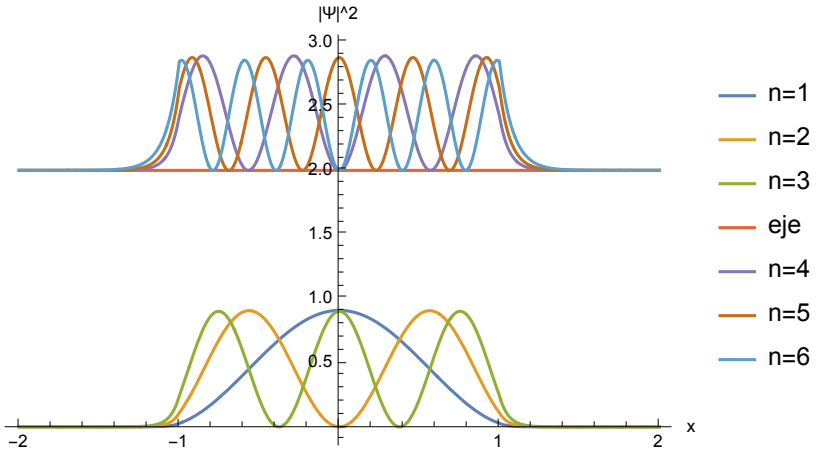
In[•]:=
```
Plot[{fopozo[[1]], fopozo[[2]], fopozo[[3]], 2, fopozo[[4]] + 2,
  fopozo[[5]] + 2, fopozo[[6]] + 2}, {x, -2, 2}, AxesLabel → {"x", "Ψ"},
 PlotLegends → {"n=1", "n=2", "n=3", "eje", "n=4", "n=5", "n=6"}]
```

Out[•]=



In[•]:=
```
Plot[{fopozo[[1]]^2, fopozo[[2]]^2, fopozo[[3]]^2, 2, fopozo[[4]]^2 + 2,
  fopozo[[5]]^2 + 2, fopozo[[6]]^2 + 2}, {x, -2, 2}, AxesLabel → {"x", "|Ψ|^2"},
 PlotLegends → {"n=1", "n=2", "n=3", "eje", "n=4", "n=5", "n=6"}]
```

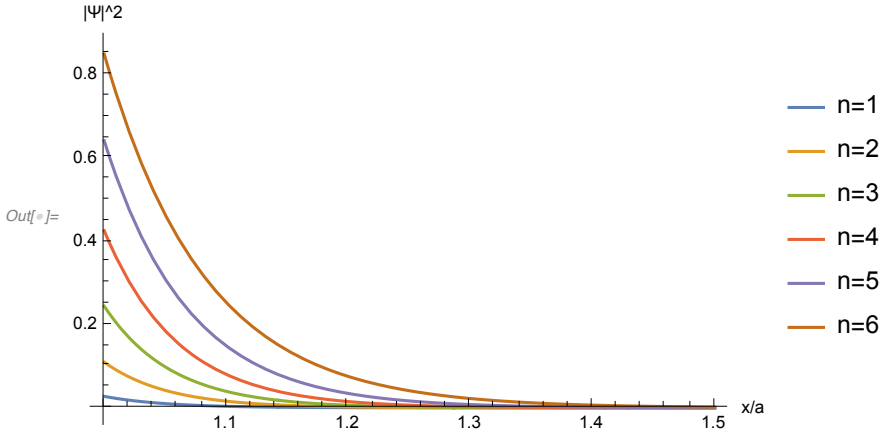
Out[•]=



El efecto tunel cuando E < Vo.

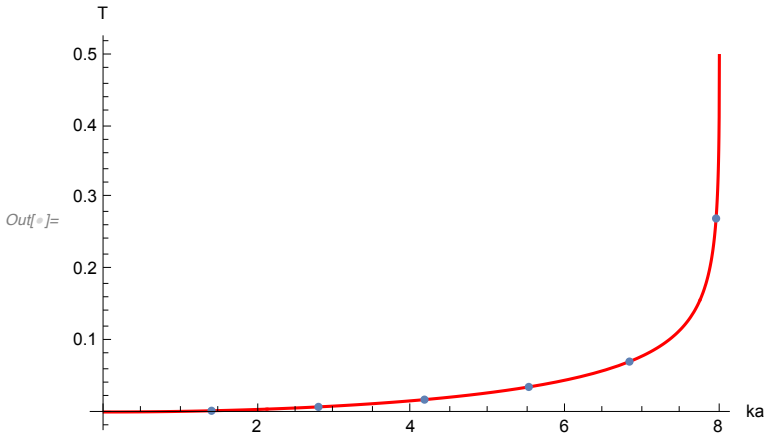
In[•]:=
```
temp = Table[fopozo[[i]]^2, {i, nepozo}];
Plot[temp, {x, 1, 1.5}, PlotRange → All, AxesLabel → {"x/a", "|Ψ|^2"},
 PlotLegends → {"n=1", "n=2", "n=3", "n=4", "n=5", "n=6"}]
```

Out[•]=



In[•]:=
```
temp = Table[
    {kspozo[[i]], 0.5 * (kspozo[[i]] / 8)^2 / (1 + Sqrt[64 - kspozo[[i]]^2])}, {i, nepozo}];
temp1 = ListPlot[temp, PlotRange → All, AxesLabel → {"ka", "T"}];
temp2 = Plot[x * x / (128 * (1 + Sqrt[64 - x * x])), {x, 0, 8},
    PlotRange → All, PlotStyle → Red, AxesLabel → {"ka", "T"}];
Show[temp2, temp1]
```

Out[•]=

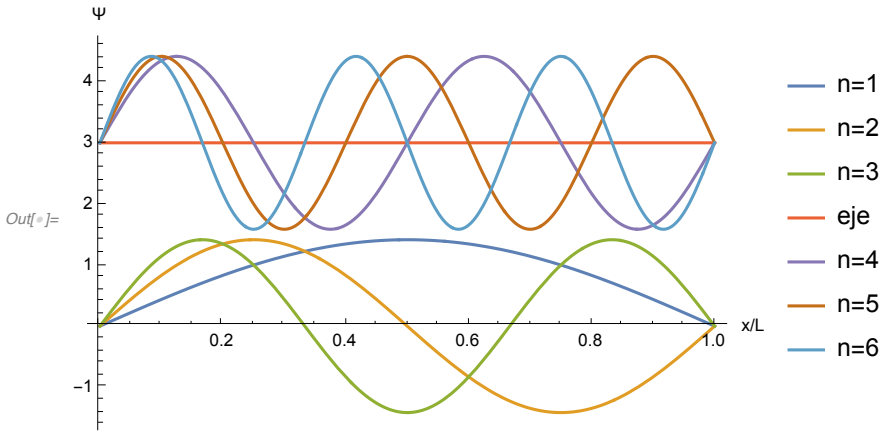


2.A.4. La partícula encerrada entre [0,L].

In[•]:=
```
fop1d[n_, x_, L_] := Sqrt[2 / L] * Sin[n * Pi * x / L];
```

In[•]:=
```
Plot[{fop1d[1, x, 1], fop1d[2, x, 1], fop1d[3, x, 1], 3, fop1d[4, x, 1] + 3,
  fop1d[5, x, 1] + 3, fop1d[6, x, 1] + 3}, {x, 0, 1}, AxesLabel → {"x/L", "Ψ"},
 PlotLegends → {"n=1", "n=2", "n=3", "eje", "n=4", "n=5", "n=6"}]
```

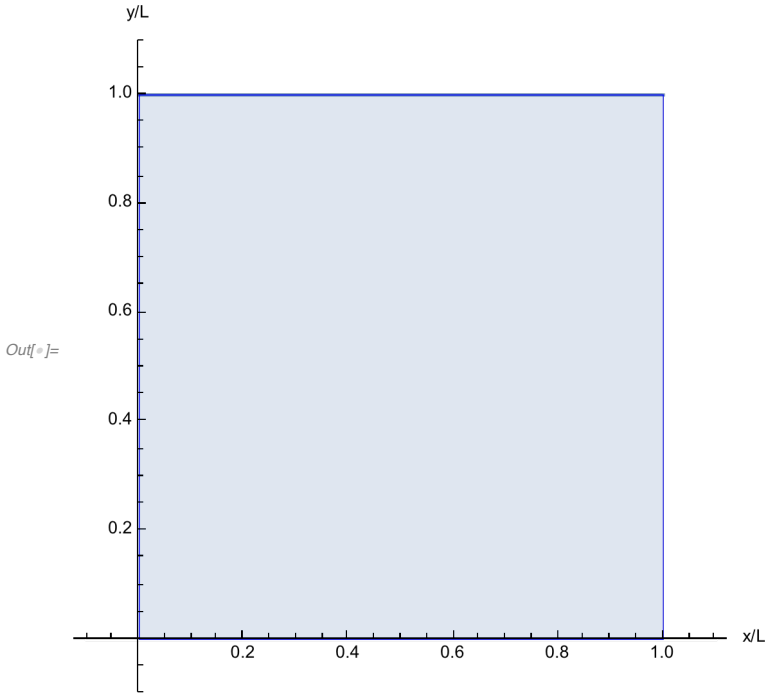
Out[•]=



2.A.5. La partícula encerrada en el cuadrado con bordes en (0,0), (0,L), (L,L), (L,0).

In[•]:=
```
Show[Plot[0, {x, -0.1, 1.1}, PlotRange → {-0.1, 1.1},
  AspectRatio → 1, AxesLabel → {"x/L", "y/L"}, PlotStyle → White],
 Plot[1, {x, 0, 1}, Filling → Axis],
 Graphics[{Blue, Line[{{0, 0}, {0, 1}, {1, 1}, {1, 0}, {0, 0}}]}]]
```

Out[•]=



El espectro.

In[•]:=
```
edo[x_, e_, xo_] := If[x ≥ xo && x ≤ xo + 1, e];
```

```
Print["Energía, E(nx,ny):"]
TableForm[Table[i * i + j * j, {i, 7}, {j, 7}],
 TableHeadings → {Table[i, {i, 7}], Table[i, {i, 7}]}]
```

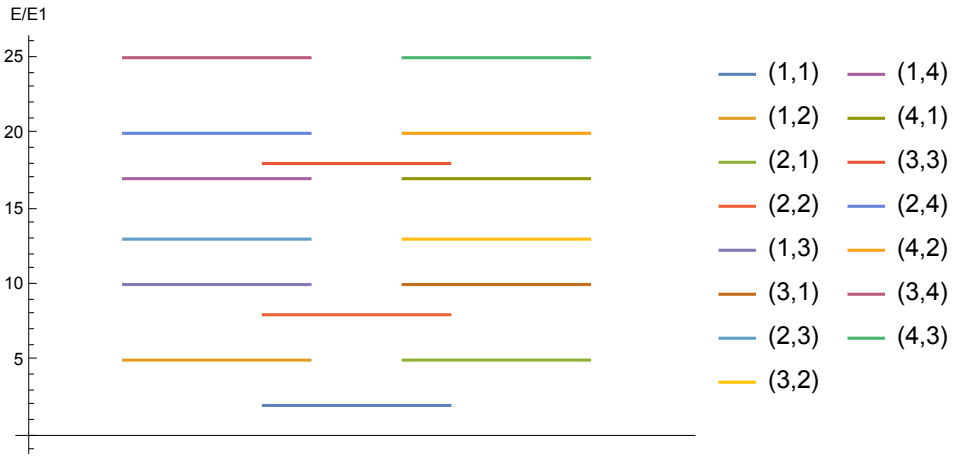
```
Energía, E(nx,ny):
```

Out[•]//TableForm=

	1	2	3	4	5	6	7
1	2	5	10	17	26	37	50
2	5	8	13	20	29	40	53
3	10	13	18	25	34	45	58
4	17	20	25	32	41	52	65
5	26	29	34	41	50	61	74
6	37	40	45	52	61	72	85
7	50	53	58	65	74	85	98

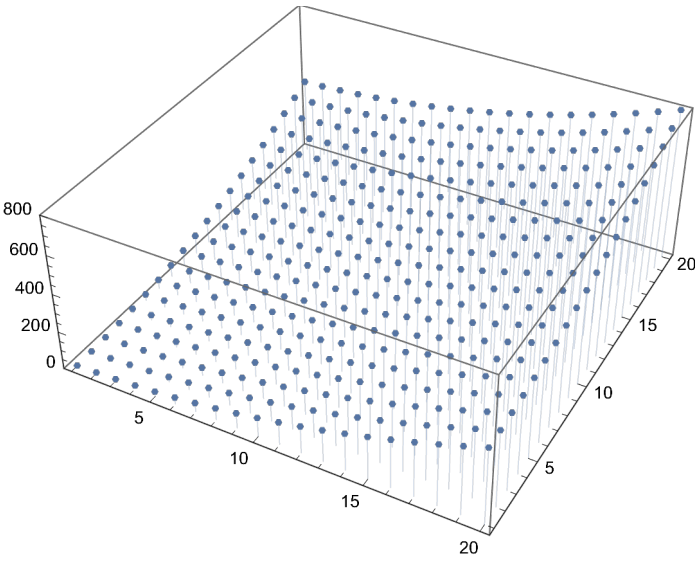
In[•]:=
```
Plot[{edo[x, 2, 1.25], edo[x, 5, 0.5], edo[x, 5, 2],
  edo[x, 8, 1.25], edo[x, 10, 0.5], edo[x, 10, 2], edo[x, 13, 0.5],
  edo[x, 13, 2], edo[x, 17, 0.5], edo[x, 17, 2], edo[x, 18, 1.25],
  edo[x, 20, 0.5], edo[x, 20, 2], edo[x, 25, 0.5], edo[x, 25, 2]},
 {x, 0, 3.5}, AxesLabel → "E/E1", Ticks → {False, True},
 PlotLegends → {"(1,1)", "(1,2)", "(2,1)", "(2,2)", "(1,3)", "(3,1)", "(2,3)",
   "(3,2)", "(1,4)", "(4,1)", "(3,3)", "(2,4)", "(4,2)", "(3,4)", "(4,3)"}]
```

Out[•]=



In[•]:=
```
ListPointPlot3D[
 Flatten[Table[{i, j, i * i + j * j}, {i, 20}, {j, 20}], 1], Filling → Bottom]
```

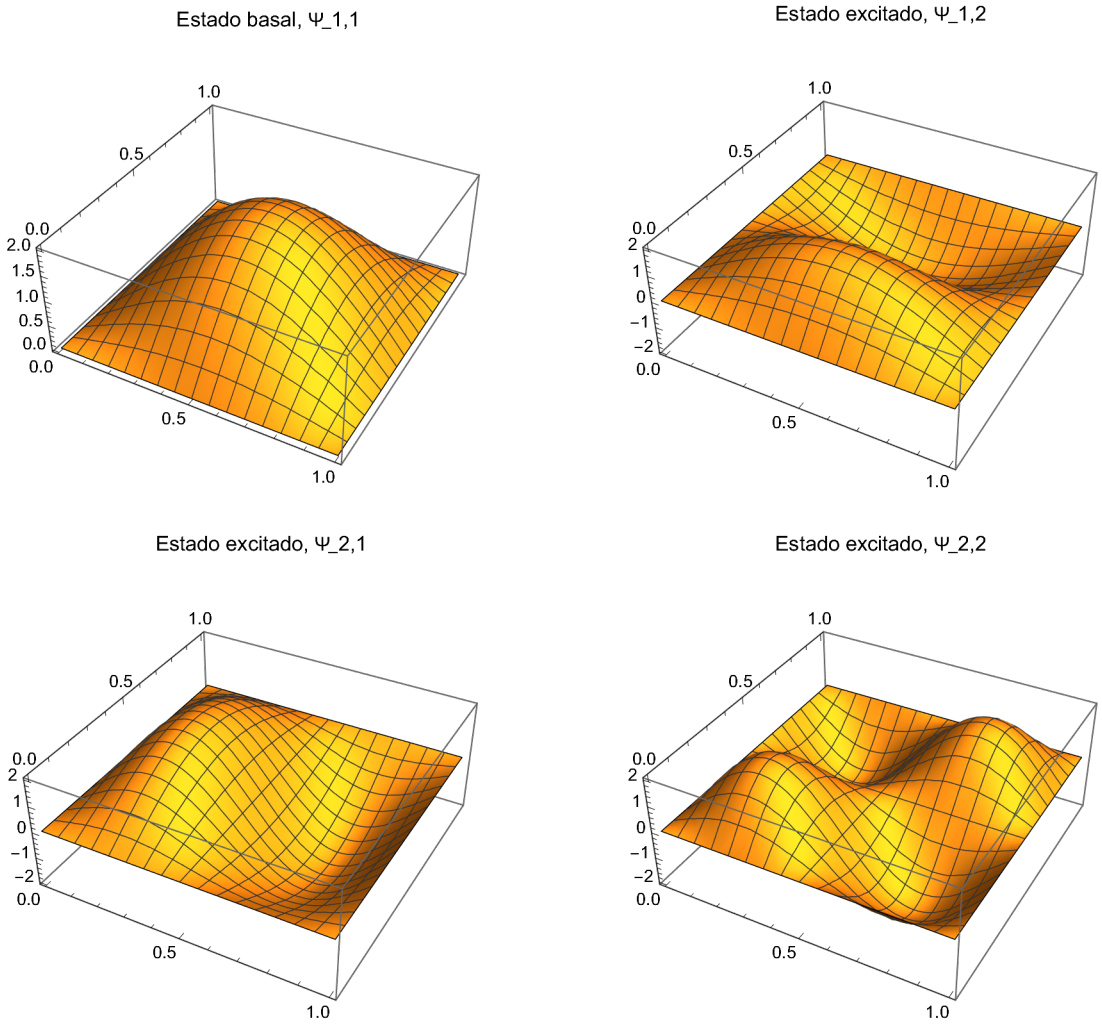
Out[•]=



Las funciones de onda.

In[ ]:=
```
GraphicsGrid[{{Plot3D[fop1d[1, x, 1] * fop1d[1, y, 1], {x, 0, 1}, {y, 0, 1},
    PlotLabel → "Estado basal, Ψ_1,1"], Plot3D[fop1d[1, x, 1] * fop1d[2, y, 1],
    {x, 0, 1}, {y, 0, 1}, PlotLabel → "Estado excitado, Ψ_1,2"]},
  {Plot3D[fop1d[2, x, 1] * fop1d[1, y, 1], {x, 0, 1}, {y, 0, 1},
    PlotLabel → "Estado excitado, Ψ_2,1"], Plot3D[fop1d[2, x, 1] * fop1d[2, y, 1],
    {x, 0, 1}, {y, 0, 1}, PlotLabel → "Estado excitado, Ψ_2,2"]}}]
```

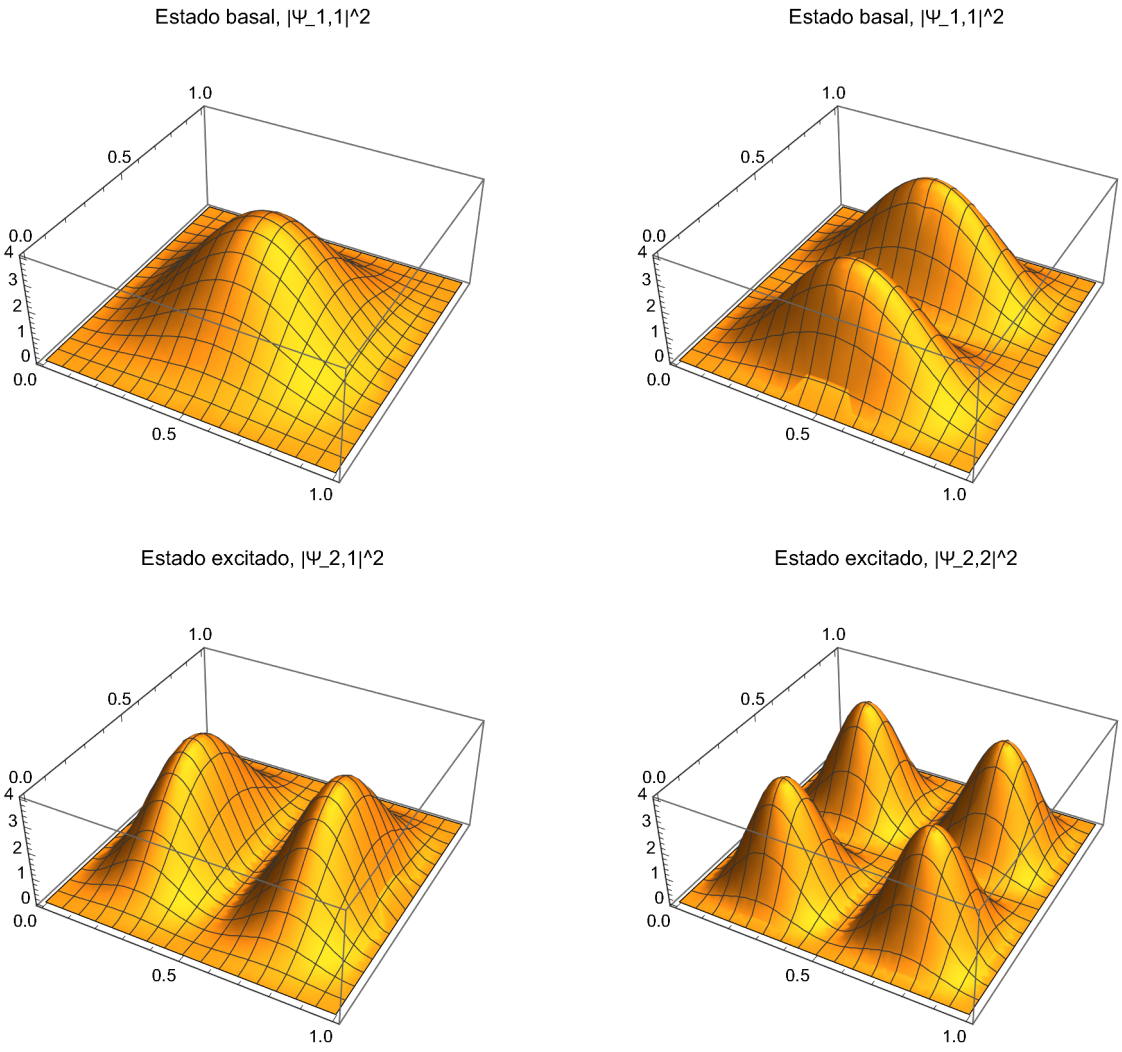
Out[ ]=



Las densidades de probabilidad.

In[•]:=
```
GraphicsGrid[
 {{Plot3D[(fop1d[1, x, 1] * fop1d[1, y, 1]) ^ 2, {x, 0, 1}, {y, 0, 1}, PlotLabel →
     "Estado basal, |Ψ_1,1|^2"], Plot3D[(fop1d[1, x, 1] * fop1d[2, y, 1]) ^ 2,
   {x, 0, 1}, {y, 0, 1}, PlotLabel → "Estado basal, |Ψ_1,1|^2"]},
  {Plot3D[(fop1d[2, x, 1] * fop1d[1, y, 1]) ^ 2, {x, 0, 1}, {y, 0, 1},
    PlotLabel → "Estado excitado, |Ψ_2,1|^2"],
   Plot3D[(fop1d[2, x, 1] * fop1d[2, y, 1]) ^ 2, {x, 0, 1}, {y, 0, 1},
    PlotLabel → "Estado excitado, |Ψ_2,2|^2"]}}]
```

Out[•]=



2.B. El movimiento vibracional.

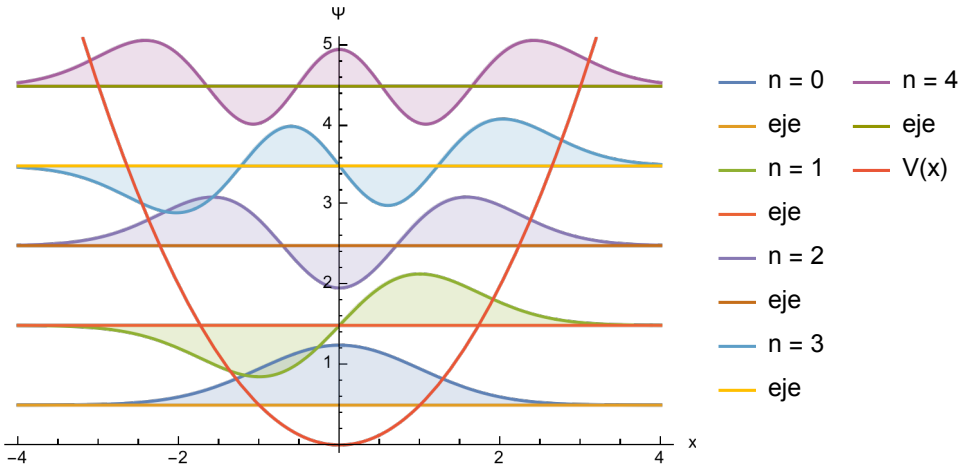
2.B.1. El oscilador armónico unidimensional.

Las funciones propias.

In[•]:=
```
fooa[n_, x_] := HermiteH[n, x] / Sqrt[Sqrt[Pi] * n! * 2^n] * Exp[-x * x / 2];
```

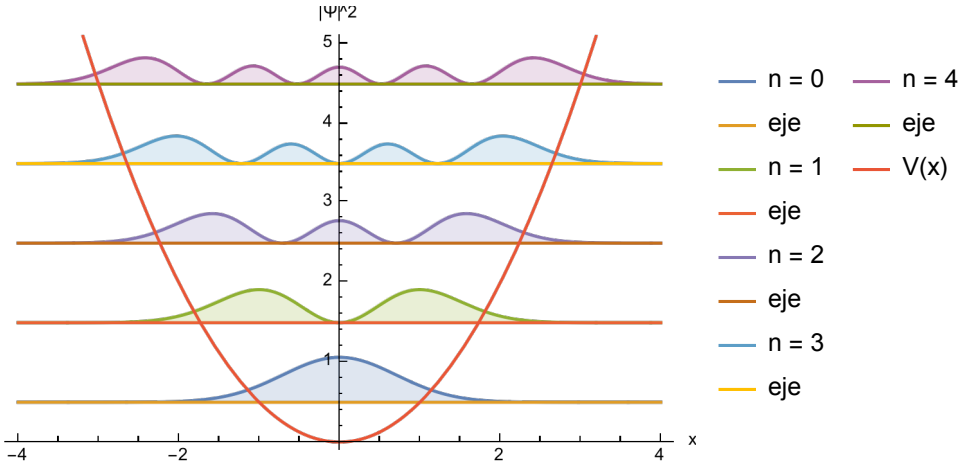
In[•]:=
```
Plot[{0.5 + fooa[0, x], 0.5, 1.5 + fooa[1, x], 1.5, 2.5 + fooa[2, x], 2.5,
  3.5 + fooa[3, x], 3.5, 4.5 + fooa[4, x], 4.5, 0.5 * x * x}, {x, -4, 4},
 PlotLegends → {"n = 0", "eje", "n = 1", "eje", "n = 2", "eje",
   "n = 3", "eje", "n = 4", "eje", "V(x)"}, PlotRange → {-0.1, 5.1},
 Filling → {1 → 0.5, 3 → 1.5, 5 → 2.5, 7 → 3.5, 9 → 4.5}, AxesLabel → {"x", "Ψ"}]
```

Out[•]=



In[•]:=
```
Plot[{0.5 + fooa[0, x]^2, 0.5, 1.5 + fooa[1, x]^2, 1.5, 2.5 + fooa[2, x]^2,
  2.5, 3.5 + fooa[3, x]^2, 3.5, 4.5 + fooa[4, x]^2, 4.5, 0.5 * x * x},
 {x, -4, 4}, PlotLegends → {"n = 0", "eje", "n = 1", "eje", "n = 2", "eje",
   "n = 3", "eje", "n = 4", "eje", "V(x)"}, PlotRange → {-0.1, 5.1},
 Filling → {1 → 0.5, 3 → 1.5, 5 → 2.5, 7 → 3.5, 9 → 4.5},
 AxesLabel → {"x", "|Ψ|^2"}]
```

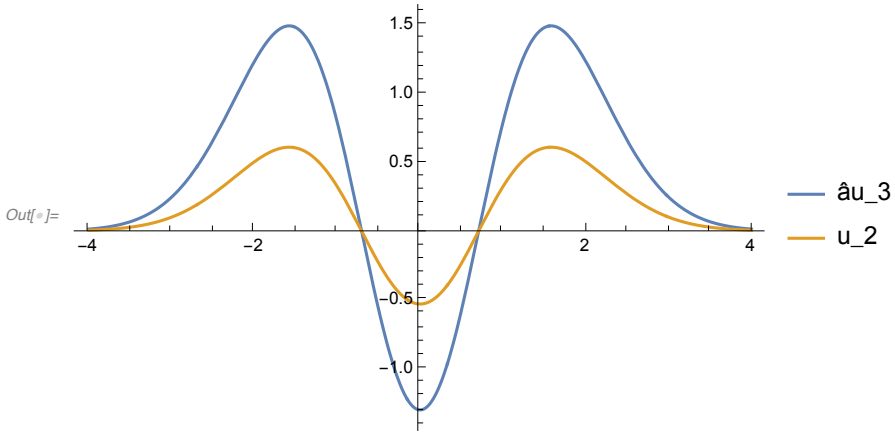
Out[•]=



La acción de los operadores de ascenso y descenso.

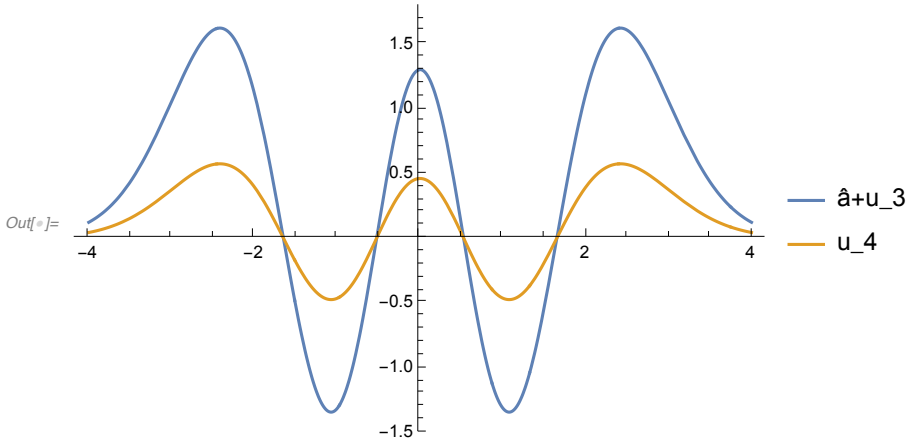
In[•]:=
```
Plot[{x * fooa[3, x] + D[fooa[3, y], y] /. y → x, fooa[2, x]},
 {x, -4, 4}, PlotLegends → {"âu_3", "u_2"}]
```

Out[•]=



In[•]:=
```
Plot[{x * fooa[3, x] - D[fooa[3, y], y] /. y → x, fooa[4, x]},
 {x, -4, 4}, PlotLegends → {"â+u_3", "u_4"}]
```

Out[•]=



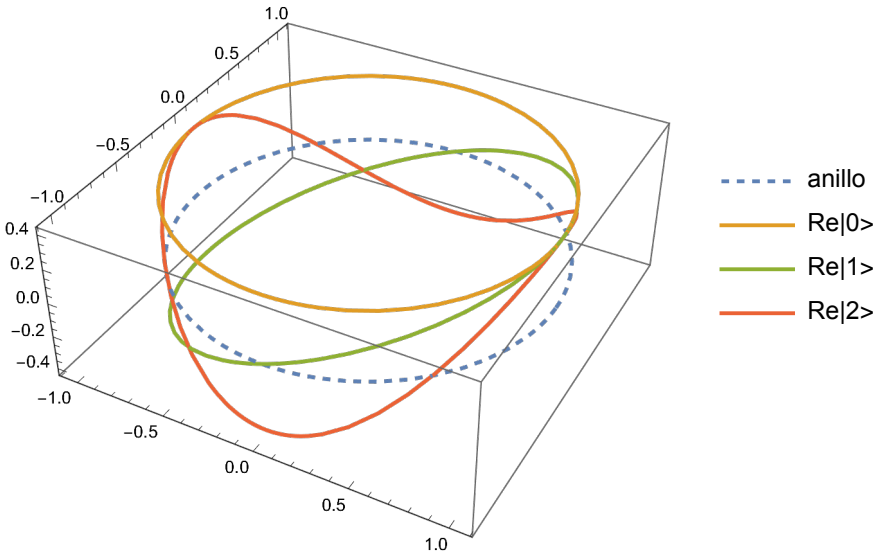
2.C. El movimiento rotacional.

2.C.1. La partícula en un anillo.

In[•]:=
```
fopan[n_, a_] = Exp[I * n * a] / Sqrt[2 * Pi];
```

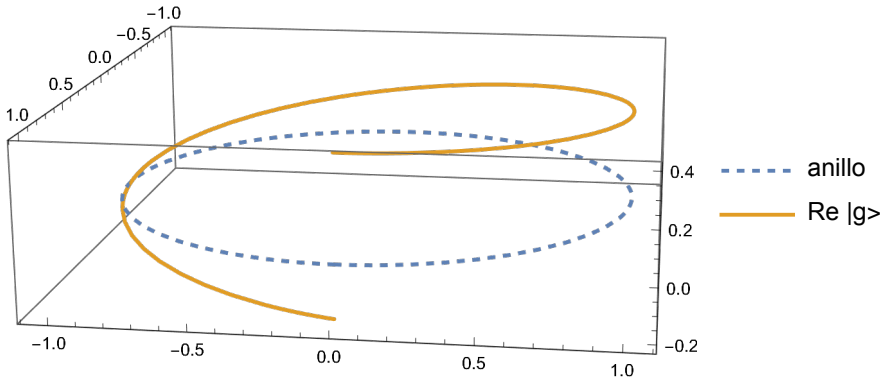
In[•]:=
```
ParametricPlot3D[{{Cos[a], Sin[a], 0}, {Cos[a], Sin[a], Re[fopan[0, a]]},
  {Cos[a], Sin[a], Re[fopan[1, a]]}, {Cos[a], Sin[a], Re[fopan[2, a]]}},
 {a, 0, 2 * Pi}, PlotStyle → { Dashed, Thick, Thick, Thick},
 PlotLegends → {"anillo", "Re|0>", "Re|1>", "Re|2>"}]
```

Out[•]=



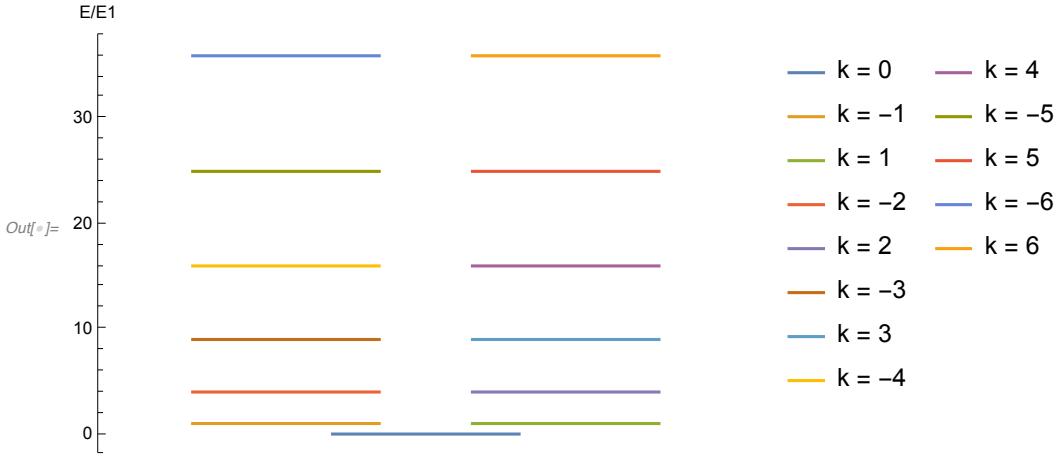
In[•]:=
```
ParametricPlot3D[{{Cos[a], Sin[a], 0}, {Cos[a], Sin[a], Re[fopan[1 / 3, a]]}},
 {a, 0, 2 * Pi}, PlotStyle → { Dashed, Thick, Thick, Thick},
 PlotLegends → {"anillo", "Re |g>"}]
```

Out[•]=



In[•]:=
```
Plot[{edo[x, 0, 1.25], edo[x, 1, 0.5], edo[x, 1, 2], edo[x, 4, 0.5],
  edo[x, 4, 2], edo[x, 9, 0.5], edo[x, 9, 2], edo[x, 16, 0.5], edo[x, 16, 2],
  edo[x, 25, 0.5], edo[x, 25, 2], edo[x, 36, 0.5], edo[x, 36, 2]},
 {x, 0, 3.5}, AxesLabel → "E/E1", PlotLegends →
  {"k = 0", "k = -1", "k = 1", "k = -2", "k = 2", "k = -3", "k = 3", "k = -4",
   "k = 4", "k = -5", "k = 5", "k = -6", "k = 6"}, Axes → {False, True}]
```

Out[•]=

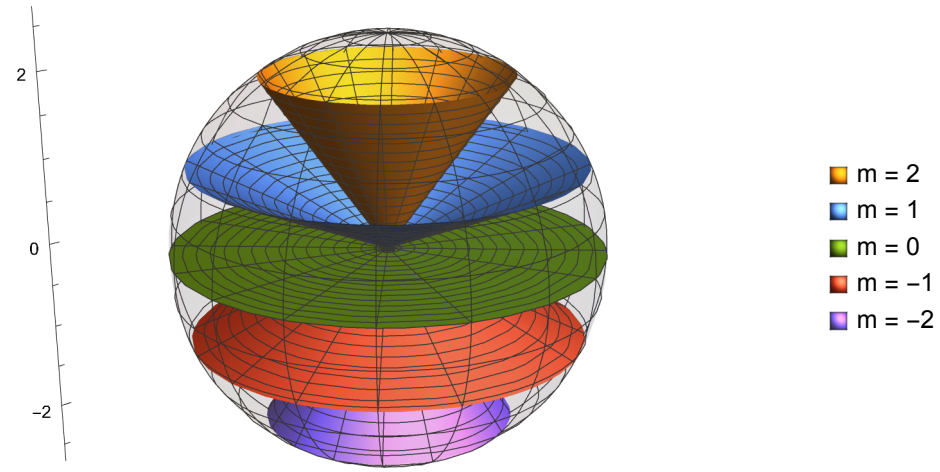


2.C.2. El momento angular.

Las componentes del momento angular.

In[•]:=
```
Show[ParametricPlot3D[
  {{r * Sin[ArcCos[2 / Sqrt[6]]] * Cos[a], r * Sin[ArcCos[2 / Sqrt[6]]] * Sin[a],
    r * 2 / Sqrt[6]}, {r * Sin[ArcCos[1 / Sqrt[6]]] * Cos[a],
    r * Sin[ArcCos[1 / Sqrt[6]]] * Sin[a], r / Sqrt[6]}, {r * Cos[a], r * Sin[a], 0},
   {r * Sin[ArcCos[-1 / Sqrt[6]]] * Cos[a], r * Sin[ArcCos[-1 / Sqrt[6]]] * Sin[a],
    -r / Sqrt[6]}, {r * Sin[ArcCos[-2 / Sqrt[6]]] * Cos[a],
    r * Sin[ArcCos[-2 / Sqrt[6]]] * Sin[a], -r * 2 / Sqrt[6]}}, {r, 0, Sqrt[6]},
  {a, 0, 2 * Pi}, PlotLegends → {"m = 2", "m = 1", "m = 0", "m = -1", "m = -2"},
  Ticks → {False, False, True}, Axes → {False, False, True}, Boxed → False],
 SphericalPlot3D[Sqrt[6], a, b, PlotStyle → Opacity[0.1, Gray]],
 PlotRange → All]
```

Out[•]=

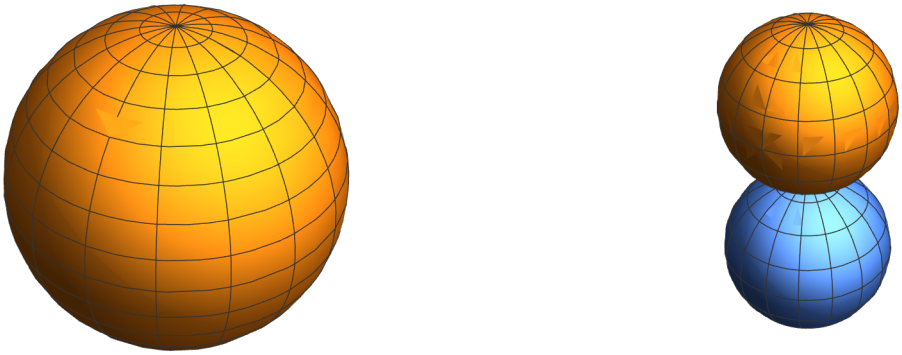


Las funciones propias.

In[ ]:=
```
GraphicsGrid[
 {{SphericalPlot3D[SphericalHarmonicY[0, 0, a, b], a, b, PlotLabel → "| 0 0 >",
    Axes → False, Boxed → False], SphericalPlot3D[
    {SphericalHarmonicY[1, 0, a, b], -SphericalHarmonicY[1, 0, a, b]}, a, b,
    PlotLabel → "| 1 0 >", Axes → False, Boxed → False]}, {SphericalPlot3D[
    {If[SphericalHarmonicY[2, 0, a, b] ≥ 0, SphericalHarmonicY[2, 0, a, b]],
     If[SphericalHarmonicY[2, 0, a, b] < 0, -SphericalHarmonicY[2, 0, a, b]]}, a,
    b, PlotLabel → "| 2 0 >", Axes → False, Boxed → False], SphericalPlot3D[
    {SphericalHarmonicY[3, 0, a, b], -SphericalHarmonicY[3, 0, a, b]},
    a, b, PlotLabel → "| 3 0 >", Axes → False, Boxed → False]}}]
```

| 0 0 >

| 1 0 >



Out[•]=

| 2 0 >

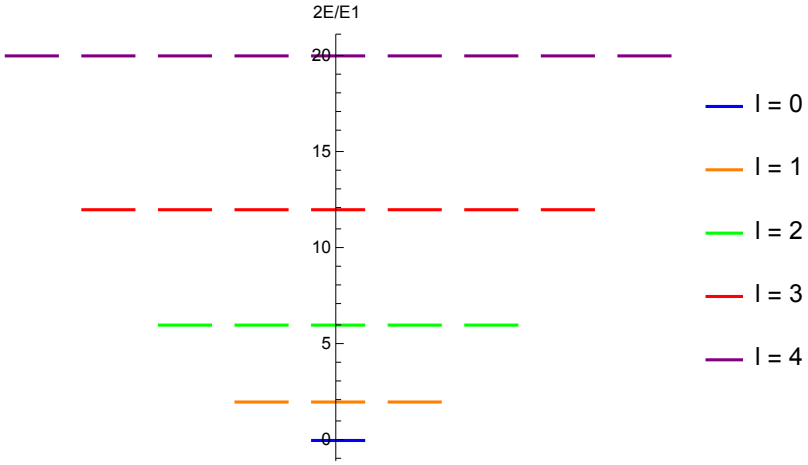
| 3 0 >

2.C.3. El rotor rígido.

In[•]:= `edorr[l_, x_] := Table[edo[x, l * (l + 1), -0.5 + (m - l - 1) * 1.5], {m, 2 * l + 1}];`

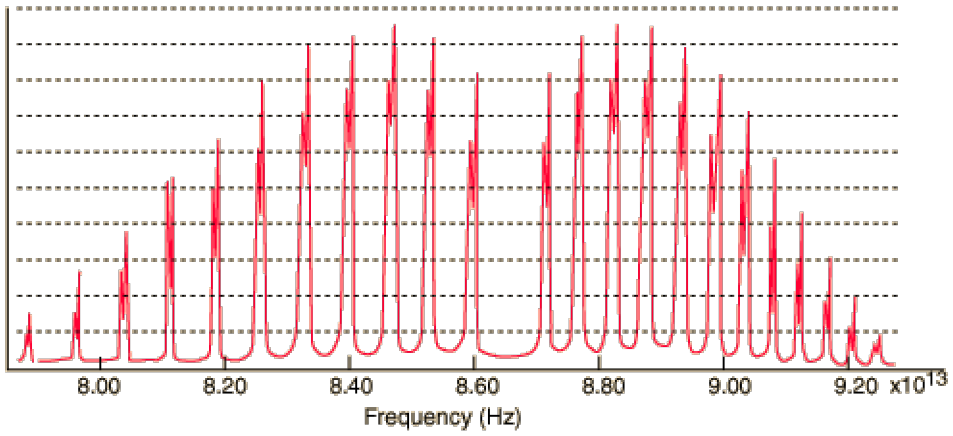
In[•]:=
```
Show[Plot[Evaluate[edorr[0, y]], {y, -7, 7}, PlotRange → All, PlotStyle → Blue,
  PlotLegends → {"l = 0"}, Axes → {False, True}, AxesLabel → "2E/E1"],
 Plot[Evaluate[edorr[1, y]], {y, -7, 7}, PlotRange → All, PlotStyle → Orange,
  PlotLegends → {"l = 1"}], Plot[Evaluate[edorr[2, y]], {y, -7, 7},
  PlotRange → All, PlotStyle → Green, PlotLegends → {"l = 2"}],
 Plot[Evaluate[edorr[3, y]], {y, -7, 7}, PlotRange → All, PlotStyle → Red,
  PlotLegends → {"l = 3"}], Plot[Evaluate[edorr[4, y]], {y, -7, 7},
  PlotRange → All, PlotStyle → Purple, PlotLegends → {"l = 4"}]]
```

Out[•]=



In[•]:=
```
Import["pc/misdocum/doc/qc/material/hclrotspec.gif"]
```

Out[•]=



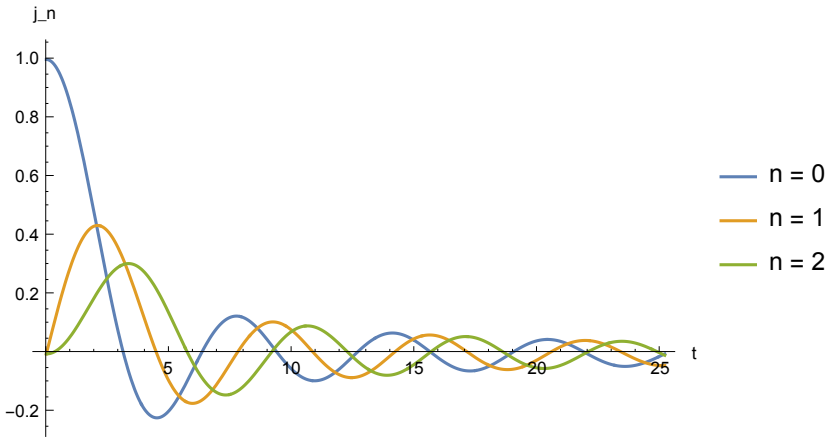
2.C.4. Los potenciales centrales: la partícula encerrada en una esfera.

Las funciones.

Las funciones esféricas de Bessel y sus raíces.

In[•]:=
```
Plot[{SphericalBesselJ[0, z], SphericalBesselJ[1, z], SphericalBesselJ[2, z]},
 {z, 0, 8 * Pi}, AxesLabel → {"t", "j_n"}, PlotRange → All,
 PlotLegends → Table["n = " <> ToString[n], {n, 0, 2}]]
```

Out[•]=



In[•]:=
```
TableForm[Table[zsb[j, i], {i, 20}, {j, 0, 7}], TableHeadings →
 {Table["x" <> ToString[i], {i, 20}], Table["j" <> ToString[j], {j, 0, 7}]}]
```

Out[•]//TableForm=

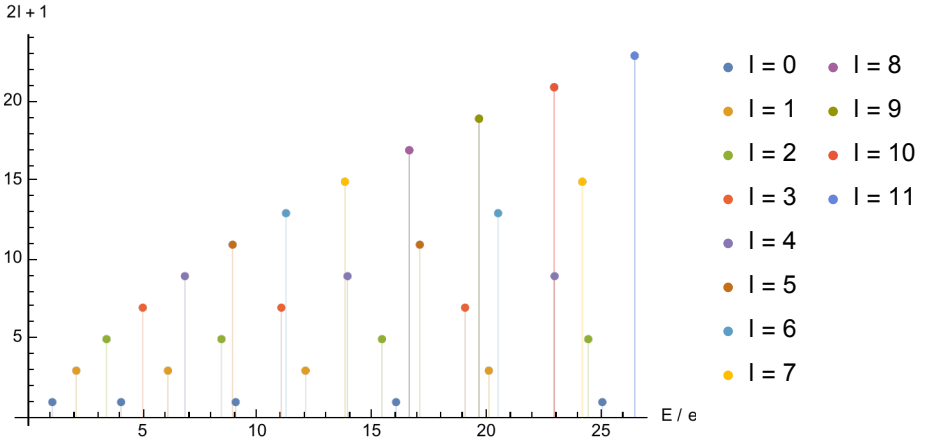
	j0	j1	j2	j3	j4	j5	j6
x1	3.14159	4.49341	5.76346	6.98793	8.18256	9.35581	10.5128
x2	6.28319	7.72525	9.09501	10.4171	11.7049	12.9665	14.2074
x3	9.42478	10.9041	12.3229	13.698	15.0397	16.3547	17.648
x4	12.5664	14.0662	15.5146	16.9236	18.3013	19.6532	20.9835
x5	15.708	17.2208	18.689	20.1218	21.5254	22.9046	24.2628
x6	18.8496	20.3713	21.8539	23.3042	24.7276	26.1278	27.5079
x7	21.9911	23.5195	25.0128	26.4768	27.9156	29.3326	30.7304
x8	25.1327	26.6661	28.1678	29.6426	31.0939	32.5247	33.9371
x9	28.2743	29.8116	31.3201	32.8037	34.2654	35.7076	37.1323
x10	31.4159	32.9564	34.4705	35.9614	37.4317	38.8836	40.3189
x11	34.5575	36.1006	37.6194	39.1165	40.5942	42.0544	43.4988
x12	37.6991	39.2444	40.7671	42.2695	43.7536	45.2211	46.6733
x13	40.8407	42.3879	43.914	45.421	46.9106	48.3844	49.8437
x14	43.9823	45.5311	47.0601	48.5711	50.0657	51.5451	53.0105
x15	47.1239	48.6741	50.2057	51.7202	53.2191	54.7035	56.1745
x16	50.2655	51.817	53.3508	54.8685	56.3712	57.8601	59.336
x17	53.4071	54.9597	56.4956	58.016	59.5222	61.0151	62.4956
x18	56.5487	58.1023	59.64	61.1629	62.6722	64.1688	65.6534
x19	59.6903	61.2447	62.7841	64.3093	65.8215	67.3213	68.8097
x20	62.8319	64.3871	65.9279	67.4553	68.97	70.4729	71.9647

El espectro.

El grado de degeneración de cada nivel es 2l + 1.

In[•]:=
```
temp = {5, 4, 4, 3, 3, 2, 2, 2, 1, 1, 1, 1};
temp0 = Table[
   Table[{(zsb[l, n] / Pi) ^ 2, 2 * l + 1}, {n, temp[[l + 1]]}], {l, 0, Length[temp] - 1}];
ListPlot[temp0, Filling → Axis, AxesLabel → {"E / e", "2l + 1"},
 PlotLegends → Table["l = " <> ToString[l], {l, 0, Length[temp] - 1}]]
```

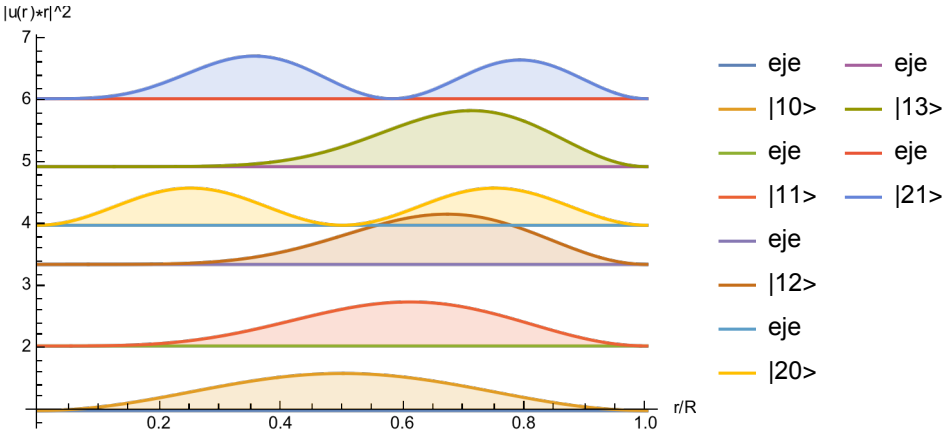
Out[•]=



Las densidades de probabilidad radial.

In[•]:=
```
Plot[{(zsb[0, 1] / Pi) ^ 2, 0.3 * (r * radps[1, 0, r]) ^ 2 + (zsb[0, 1] / Pi) ^ 2,
   (zsb[1, 1] / Pi) ^ 2,  0.3 * (r * radps[1, 1, r]) ^ 2 + (zsb[1, 1] / Pi) ^ 2,
   (zsb[2, 1] / Pi) ^ 2, 0.3 * (r * radps[1, 2, r]) ^ 2 + (zsb[2, 1] / Pi) ^ 2,
   (zsb[0, 2] / Pi) ^ 2, 0.3 * (r * radps[2, 0, r]) ^ 2 + (zsb[0, 2] / Pi) ^ 2,
   (zsb[3, 1] / Pi) ^ 2, 0.3 * (r * radps[1, 3, r]) ^ 2 + (zsb[3, 1] / Pi) ^ 2,
   (zsb[1, 2] / Pi) ^ 2,  0.3 * (r * radps[2, 1, r]) ^ 2 + (zsb[1, 2] / Pi) ^ 2}, {r, 0, 1},
 Filling → {2 → (zsb[0, 1] / Pi) ^ 2, 4 → (zsb[1, 1] / Pi) ^ 2, 6 → (zsb[2, 1] / Pi) ^ 2,
   8 → (zsb[0, 2] / Pi) ^ 2, 10 → (zsb[3, 1] / Pi) ^ 2, 12 → (zsb[1, 2] / Pi) ^ 2},
 AxesLabel → {"r/R", "|u(r)*r|^2"}, PlotLegends → {"eje", "|10>", "eje",
   "|11>", "eje", "|12>", "eje", "|20>", "eje", "|13>", "eje", "|21>"}]
```

Out[•]=



La normalización.

El valor promedio de la distancia al centro, < r > .

In[•]:=
```
TableForm[Table[NIntegrate[radps[n, l, t]^2 * t^3, {t, 0, 1}], {n, 6}, {l, 0, 4}],
 TableHeadings →
  {Table["n=" <> ToString[i], {i, 6}], Table["l=" <> ToString[j], {j, 0, 4}]}]
```

Out[•]//TableForm=

	l=0	l=1	l=2	l=3	l=4
n=1	0.5	0.591667	0.647534	0.68628	0.715214
n=2	0.5	0.539373	0.573883	0.602798	0.62714
n=3	0.5	0.522539	0.545824	0.567391	0.586855
n=4	0.5	0.514797	0.53164	0.54828	0.564023
n=5	0.5	0.510542	0.523346	0.536584	0.54955
n=6	0.5	0.507932	0.518029	0.52883	0.539693

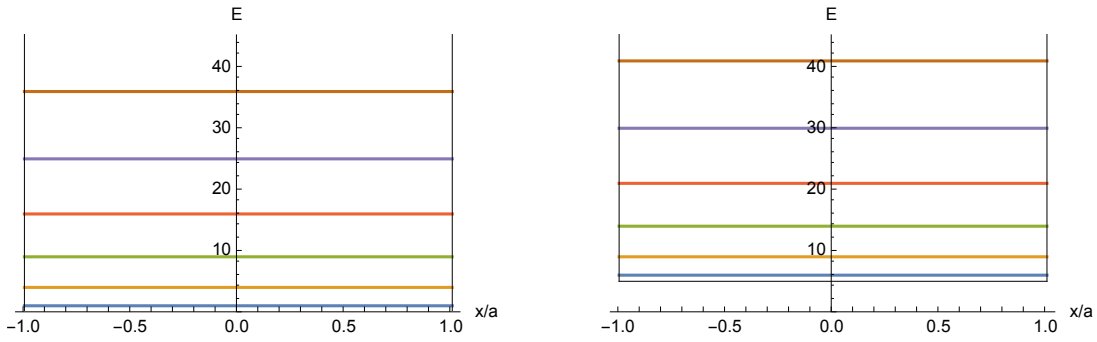
2.D. La teoría de perturbaciones.

2.D.1. La teoría de perturbaciones independiente del tiempo.

La partícula encerrada con un potencial constante.

In[•]:=
```
GraphicsGrid[{{ Show[Plot[{1, 4, 9, 16, 25, 36}, {x, -1, 1}, PlotRange → {0, 45},
      AxesLabel → {"x/a", "E"}], Graphics[{Black, Line[{{-1, 0}, {1, 0}}]}],
    Graphics[{Black, Line[{{-1, 0}, {-1, 52}}]}],
    Graphics[{Black, Line[{{1, 0}, {1, 52}}]}]],
   Show[Plot[{6, 9, 14, 21, 30, 41}, {x, -1, 1}, PlotRange → {0, 45},
     AxesLabel → {"x/a", "E"}], Graphics[{Black, Line[{{-1, 5}, {1, 5}}]}],
    Graphics[{Black, Line[{{-1, 5}, {-1, 52}}]}],
    Graphics[{Black, Line[{{1, 5}, {1, 52}}]}]]}}]
```

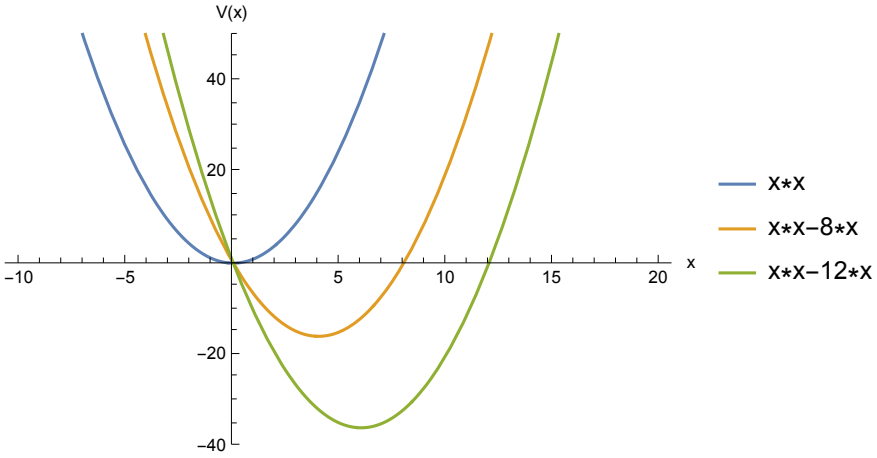
Out[•]=



El oscilador armónico en presencia de una fuerza constante.

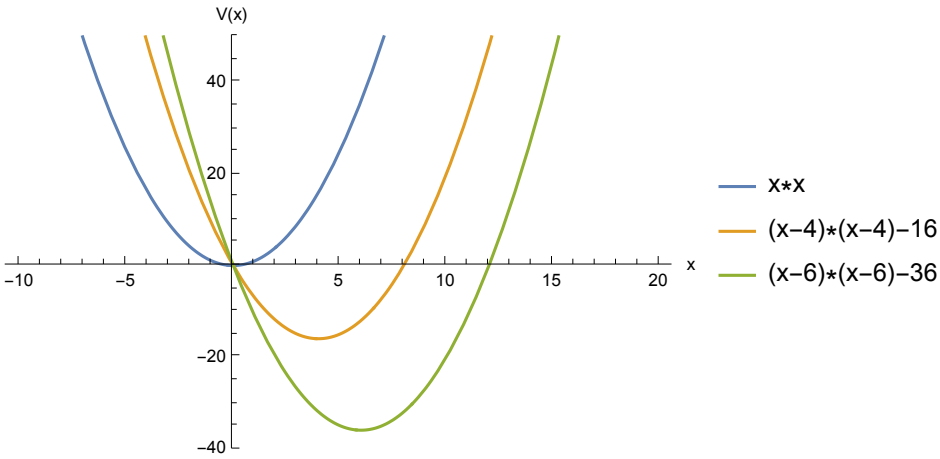
In[•]:=
```
Plot[{x * x, x * x - 8 * x, x * x - 12 * x}, {x, -10, 20}, PlotRange → {-40, 50},
 AxesLabel → {"x", "V(x)"}, PlotLegends → {"x*x", "x*x-8*x", "x*x-12*x"}]
```

Out[•]=



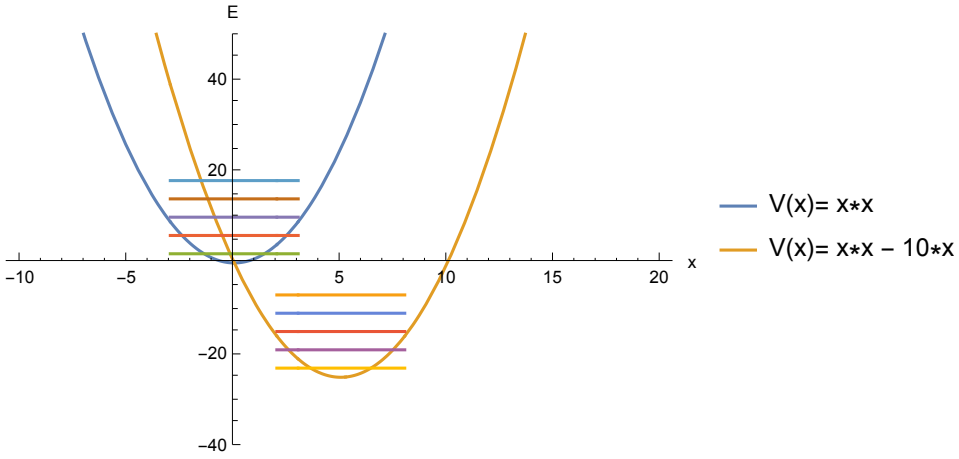
In[•]:=
```
Plot[{x * x, (x - 4) * (x - 4) - 16, (x - 6) * (x - 6) - 36},
 {x, -10, 20}, PlotRange → {-40, 50}, AxesLabel → {"x", "V(x)"},
 PlotLegends → {"x*x", "(x-4)*(x-4)-16", "(x-6)*(x-6)-36"}]
```

Out[•]=



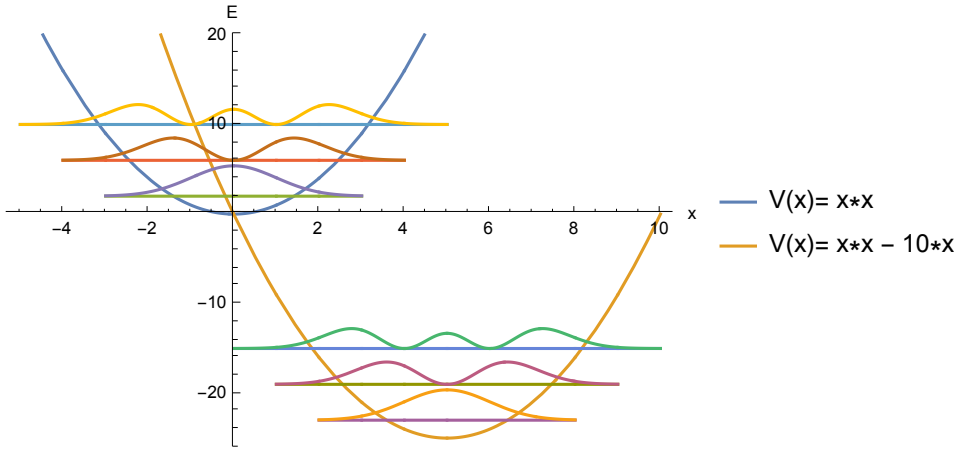
In[•]:=
```
Plot[{x * x, x * x - 10 * x, If[x > -3 && x < 3, 2],
  If[x > -3 && x < 3, 6], If[x > -3 && x < 3, 10], If[x > -3 && x < 3, 14],
  If[x > -3 && x < 3, 18], If[x > 2 && x < 8, -23], If[x > 2 && x < 8, -19], ,
  If[x > 2 && x < 8, -15], If[x > 2 && x < 8, -11], If[x > 2 && x < 8, -7]},
 {x, -10, 20}, PlotRange → {-40, 50}, AxesLabel → {"x", "E"},
 PlotLegends → {"V(x)= x*x", "V(x)= x*x - 10*x"}]
```

Out[•]=



In[•]:=
```
Plot[{x * x, x * x - 10 * x, If[x > -3 && x < 3, 2],
  If[x > -4 && x < 4, 6], If[x > -3 && x < 3, 6 * fooa[0, x / Sqrt[2]] ^ 2 + 2],
  If[x > -4 && x < 4, 6 * fooa[1, x / Sqrt[2]] ^ 2 + 6], If[x > -5 && x < 5, 10],
  If[x > -5 && x < 5, 6 * fooa[2, x / Sqrt[2]] ^ 2 + 10],
  If[x > 2 && x < 8, -23], If[x > 1 && x < 9, -19], , If[x > 0 && x < 10, -15],
  If[x > 2 && x < 8, 6 * fooa[0, (x - 5) / Sqrt[2]] ^ 2 - 23],
  If[x > 1 && x < 9, 6 * fooa[1, (x - 5) / Sqrt[2]] ^ 2 - 19],
  If[x > 0 && x < 10, 6 * fooa[2, (x - 5) / Sqrt[2]] ^ 2 - 15]},
 {x, -5, 10}, PlotRange → {-26, 20}, AxesLabel → {"x", "E"},
 PlotLegends → {"V(x)= x*x", "V(x)= x*x - 10*x"}]
```

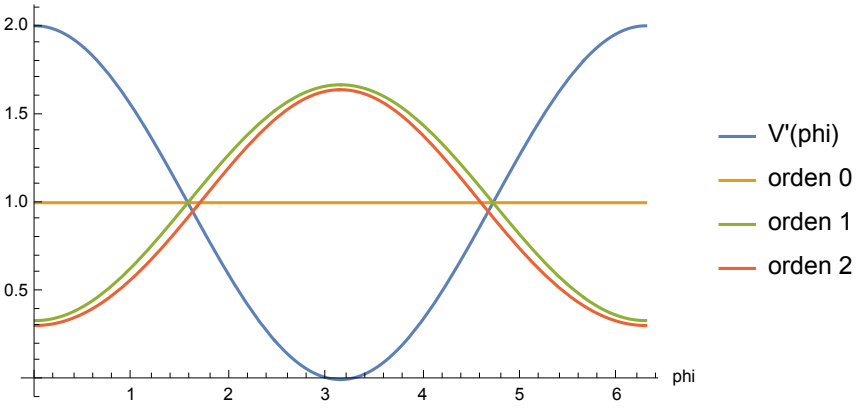
Out[•]=



La partícula en un anillo con un potencial cosenoidal.

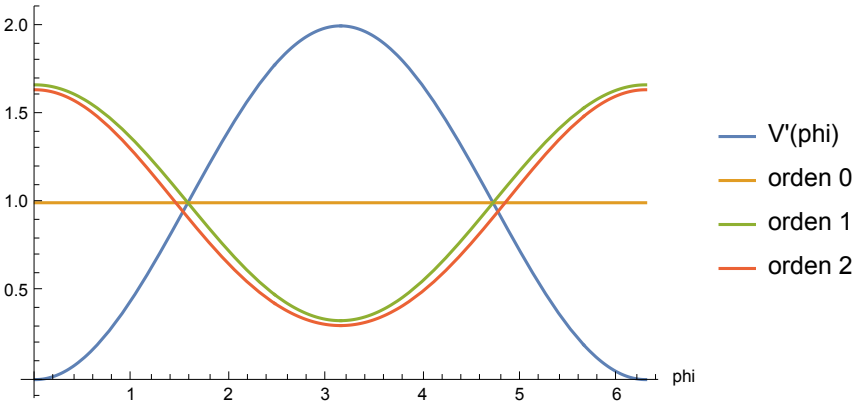
```
In[•]:= Plot[{1 + Cos[t], 1, 1 - 2 / 3 * Cos[t], 1 - 2 / 3 * Cos[t] + 1 / (4 * 9) * (Cos[2 * t] - 2)},
  {t, 0, 2 * Pi}, AxesLabel → {"phi"},
  PlotLegends → {"V'(phi)", "orden 0", "orden 1", "orden 2"}]
```

Out[•]=




```
In[•]:= Plot[{1 - Cos[t], 1, 1 + 2 / 3 * Cos[t], 1 + 2 / 3 * Cos[t] + 1 / (4 * 9) * (Cos[2 * t] - 2)},
  {t, 0, 2 * Pi}, AxesLabel → {"phi"},
  PlotLegends → {"V'(phi)", "orden 0", "orden 1", "orden 2"}]
```

Out[•]=

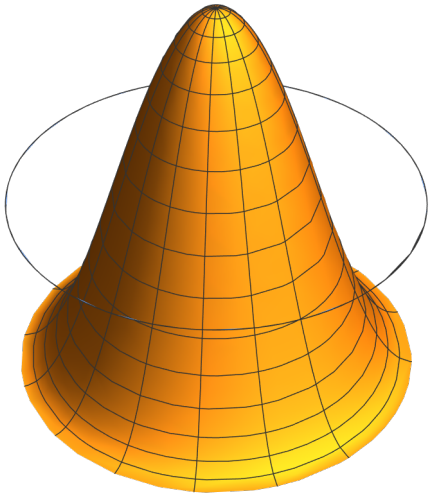


La partícula en una esfera con un potencial radial de tipo cosenoidal .

Los niveles con l = 0 no son degenerados.
Mientras que, aquellos con l > 0 tienen grado de degeneración 2l + 1.

In[]:=
```
ParametricPlot3D[{{r * Cos[a], r * Sin[a], Cos[r * Pi]}, {Cos[a], Sin[a], 0}},
 {r, 0, 1}, {a, 0, 2 * Pi}, Boxed → False, Axes → False]
```

Out[]=



Integrales para la corrección a primer orden en la energía .

In[]:=
```
TableForm[Table[NIntegrate[radps[n, l, t]^2 * t^2 * Cos[Pi * t], {t, 0, 1}],
  {n, 6}, {l, 0, 4}], TableHeadings →
  {Table["n=" <> ToString[i], {i, 6}], Table["l=" <> ToString[j], {j, 0, 4}]}]
```

Out[]//TableForm=

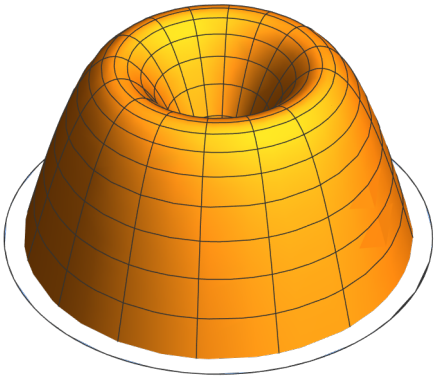
	l=0	l=1	l=2	l=3	l=4
n=1	-7.58942×10^{-16}	−0.254408	−0.409114	−0.513051	−0.587558
n=2	7.37257×10^{-17}	−0.0824195	−0.170607	−0.250223	−0.319288
n=3	0.	−0.04094	−0.0939641	−0.148635	−0.201009
n=4	-2.94903×10^{-17}	−0.024501	−0.0595651	−0.0985984	−0.138351
n=5	-3.46945×10^{-18}	−0.0163133	−0.0411527	−0.0702286	−0.101103
n=6	-3.46945×10^{-17}	−0.0116439	−0.0301417	−0.0525789	−0.0771391

La partícula en una esfera con un potencial radial de tipo sinusoidal .

Los niveles con l = 0 no son degenerados.
Mientras que aquellos con l > 0 tienen grado de degeneración 2l + 1.

In[•]:=
```
ParametricPlot3D[
 {{r * Cos[a], r * Sin[a], Sin[r * Pi]}, {1.1 * Cos[a], 1.1 Sin[a], 0}},
 {r, 0, 1}, {a, 0, 2 * Pi}, Boxed → False, Axes → False]
```

Out[•]=



Integrales para la corrección a primer orden en la energía .

In[•]:=
```
TableForm[Table[NIntegrate[radps[n, l, t]^2 * t^2 * Sin[Pi * t], {t, 0, 1}],
  {n, 6}, {l, 0, 4}], TableHeadings →
  {Table["n=" <> ToString[i], {i, 6}], Table["l=" <> ToString[j], {j, 0, 4}]}]
```

Out[•]//TableForm=

	l=0	l=1	l=2	l=3	l=4
n=1	0.848826	0.847638	0.810894	0.768607	0.728022
n=2	0.679061	0.736047	0.766232	0.777957	0.778534
n=3	0.654809	0.695453	0.727585	0.749329	0.762634
n=4	0.646725	0.675957	0.703494	0.72565	0.742311
n=5	0.64305	0.664985	0.687913	0.708219	0.725066
n=6	0.641072	0.65815	0.677305	0.695376	0.71132

2.D.2. La teoría de perturbaciones dependiente del tiempo.

La partícula encerrada en una esfera.

Las integrales dipolares.

L = 0 < = > L = 1

In[•]:=
```
TableForm[Table[NIntegrate[radps[p, 1, t] * radps[n, 0, t] * t^3, {t, 0, 1}],
  {n, 6}, {p, 5}], TableHeadings →
  {Table["n=" <> ToString[n], {n, 6}], Table["p=" <> ToString[p], {p, 5}]}]
```

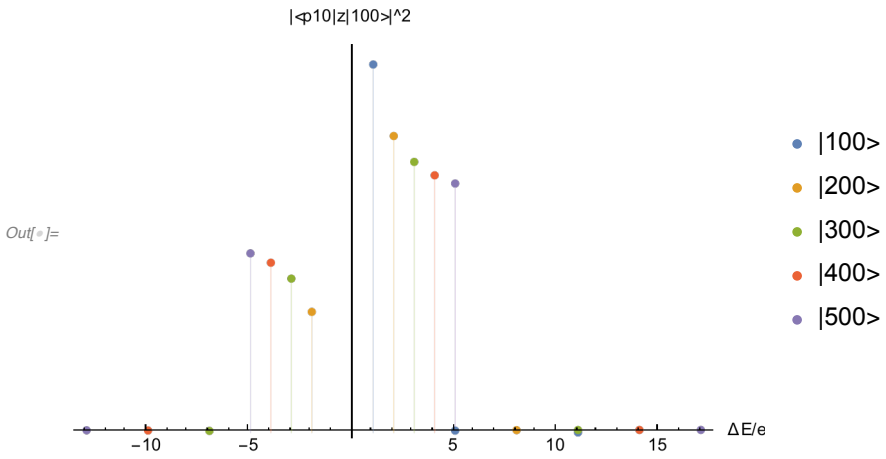
Out[•]//TableForm=

	p=1	p=2	p=3	p=4	p=5
n=1	0.530068	−0.0391283	0.0115267	−0.00500179	0.00263301
n=2	−0.303568	0.475776	−0.0434465	0.0140935	−0.00654891
n=3	0.0359589	−0.342814	0.454523	−0.0446072	0.015045
n=4	−0.0119078	0.04024	−0.360101	0.443139	−0.045034
n=5	0.00550085	−0.0138716	0.0419214	−0.369874	0.436038
n=6	−0.00301682	0.00666481	−0.0147108	0.0427823	−0.376164

Las amplitudes de la transición.

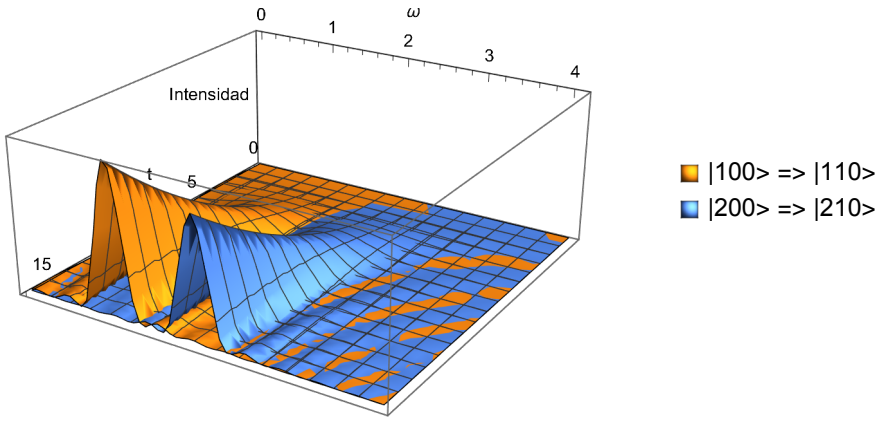
In[•]:=
```
temp = Table[{(zsb[1, p]^2 - zsb[0, 1]^2) / Pi^2,
    NIntegrate[radps[p, 1, t] * radps[1, 0, t] * t^3, {t, 0, 1}]^2}, {p, 3}];
temp = Append[{temp}, Table[{(zsb[1, p]^2 - zsb[0, 2]^2) / Pi^2,
     NIntegrate[radps[p, 1, t] * radps[2, 0, t] * t^3, {t, 0, 1}]^2}, {p, 3}]];
temp = Append[temp, Table[{(zsb[1, p]^2 - zsb[0, 3]^2) / Pi^2,
     NIntegrate[radps[p, 1, t] * radps[3, 0, t] * t^3, {t, 0, 1}]^2}, {p, 4}]];
temp = Append[temp, Table[{(zsb[1, p]^2 - zsb[0, 4]^2) / Pi^2,
     NIntegrate[radps[p, 1, t] * radps[4, 0, t] * t^3, {t, 0, 1}]^2}, {p, 2, 5}]];
temp = Append[temp, Table[{(zsb[1, p]^2 - zsb[0, 5]^2) / Pi^2,
     NIntegrate[radps[p, 1, t] * radps[5, 0, t] * t^3, {t, 0, 1}]^2}, {p, 3, 6}]];
ListPlot[temp, Filling → Axis, AxesLabel → {"ΔE/e", "|<p10|z|100>|^2"},
 Ticks → {True, False}, PlotRange → All,
 PlotLegends → {"|100>", "|200>", "|300>", "|400>", "|500>"}]
```

Out[•]=



In[]:=
```
tempw = (zsb[1, 1]^2 - zsb[0, 1]^2) / Pi^2;
temp = NIntegrate[radps[1, 1, t] * radps[1, 0, t] * t^3, {t, 0, 1}]^2;
tempv = (zsb[1, 2]^2 - zsb[0, 2]^2) / Pi^2;
tempi = NIntegrate[radps[2, 1, t] * radps[2, 0, t] * t^3, {t, 0, 1}]^2;
Plot3D[{temp * (Sin[(w - tempw) * t / 2] / (w - tempw))^2,
  tempi * (Sin[(w - tempv) * t / 2] / (w - tempv))^2}, {t, 0, 16},
 {w, 0, 2 * tempv}, PlotRange → All, AxesLabel → {"t", "ω", "Intensidad"},
 Ticks → {True, True, False}, PlotLegends → {"|100> => |110>", "|200> => |210>"}]
```

Out[]=



L = 1 <=> L = 2

In[]:=
```
TableForm[Table[NIntegrate[radps[p, 2, t] * radps[n, 1, t] * t^3, {t, 0, 1}],
  {n, 6}, {p, 5}], TableHeadings →
  {Table["n=" <> ToString[n], {n, 6}], Table["p=" <> ToString[p], {p, 5}]}]
```

Out[]//TableForm=

	p=1	p=2	p=3	p=4	p=5
n=1	0.610447	−0.0418103	0.0127766	−0.00573471	0.00310167
n=2	−0.254337	0.529446	−0.0448185	0.01463	−0.0068859
n=3	0.0342413	−0.303041	0.494906	−0.0456116	0.0153584
n=4	−0.0119632	0.038601	−0.327627	0.475527	−0.0458611
n=5	0.00572495	−0.0137012	0.0405408	−0.342597	0.463079
n=6	−0.0032222	0.00671271	−0.0145023	0.0416188	−0.352699

L = 2 <=> L = 3

```
In[•]:= TableForm[Table[NIntegrate[radps[p, 3, t] * radps[n, 2, t] * t^3, {t, 0, 1}],
          {n, 6}, {p, 5}], TableHeadings →
          {Table["n=" <> ToString[n], {n, 5}], Table["p=" <> ToString[p], {p, 6}]}]
```

Out[•]//TableForm=

	p=1	p=2	p=3	p=4	p=5
n=1	0.660813	−0.0423559	0.0132435	−0.00608609	0.00335812
n=2	−0.22137	0.569466	−0.0452723	0.0148395	−0.00705287
n=3	0.0324526	−0.273385	0.527385	−0.0460759	0.0154914
n=4	−0.0117795	0.0369976	−0.301862	0.502744	−0.0463239
n=5	0.00578701	−0.0134342	0.0391908	−0.320065	0.486469
	−0.00332282	0.00668507	−0.0142424	0.0404747	−0.332759

3. La estructura atómica.

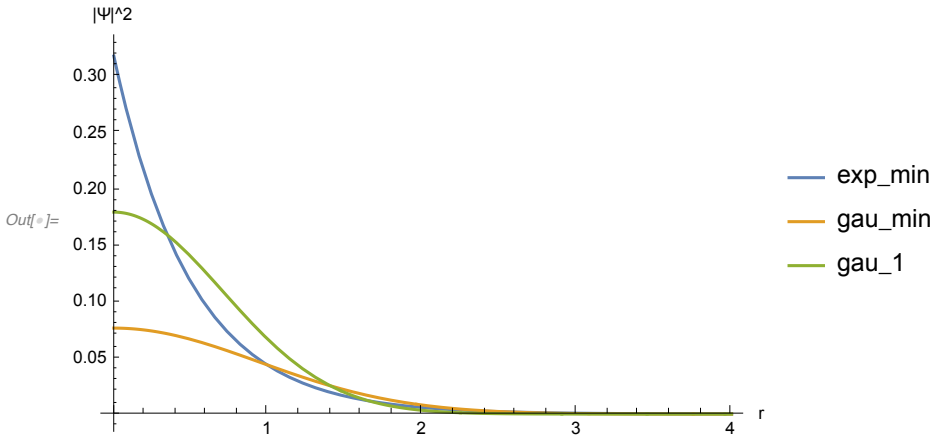
3.A. Los átomos hidrogenoides.

3.A.1. Algunos modelos para la función de onda.

```
In[•]:= prexp[a_, r_] := a^3 / Pi * Exp[-2 * a * r];
        prgau[a_, r_] := (a / Sqrt[Pi])^3 * Exp[-a * a * r * r];
```

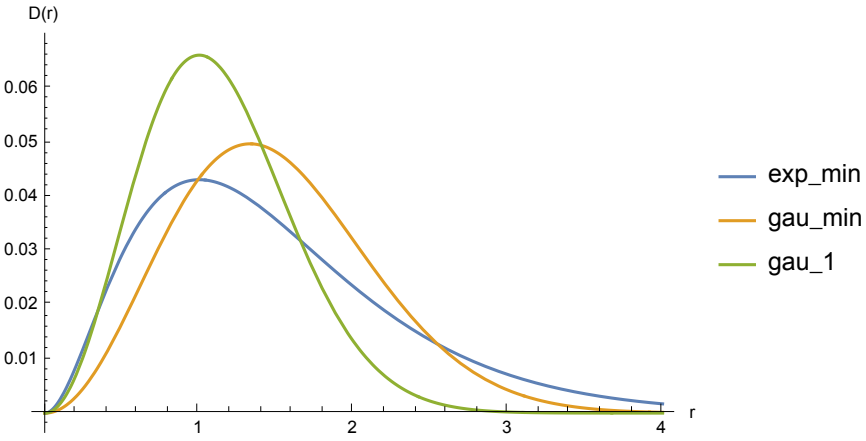
```
In[•]:= Plot[{prexp[1, r], prgau[4 / (3 * Sqrt[Pi]), r], prgau[1, r]},
         {r, 0, 4}, PlotRange → All, AxesLabel → {"r", "|Ψ|^2"},
         PlotLegends → {"exp_min", "gau_min", "gau_1"}]
```

Out[•]=



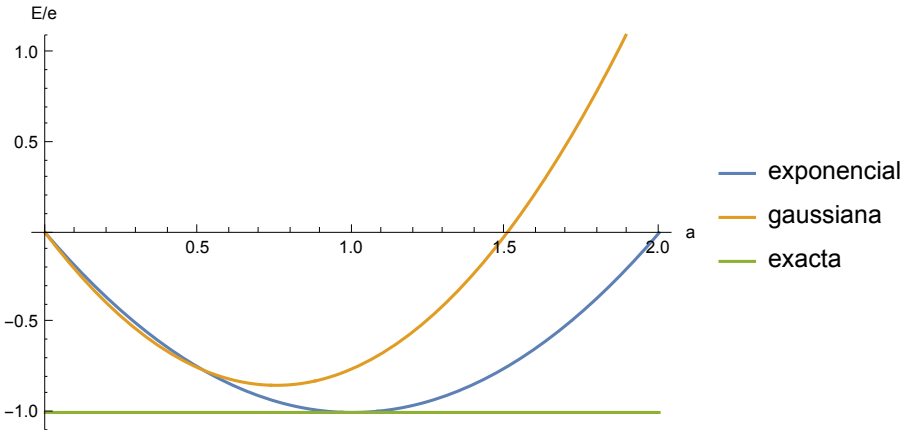
In[•]:=
```
Plot[{prexp[1, r] * r * r, prgau[4 / (3 * Sqrt[Pi]), r] * r * r, prgau[1, r] * r * r},
 {r, 0, 4}, PlotRange → All, AxesLabel → {"r", "D(r)"},
 PlotLegends → {"exp_min", "gau_min", "gau_1"}]
```

Out[•]=



In[•]:=
```
Plot[{x * x - 2 * 1 * x, 3 / 2 * x * x - 4 * 1 / Sqrt[Pi] * x, -1},
 {x, 0, 2}, PlotRange → {-1.1, 1.1}, AxesLabel → {"a", "E/e"},
 PlotLegends → {"exponencial", "gaussiana", "exacta"}]
```

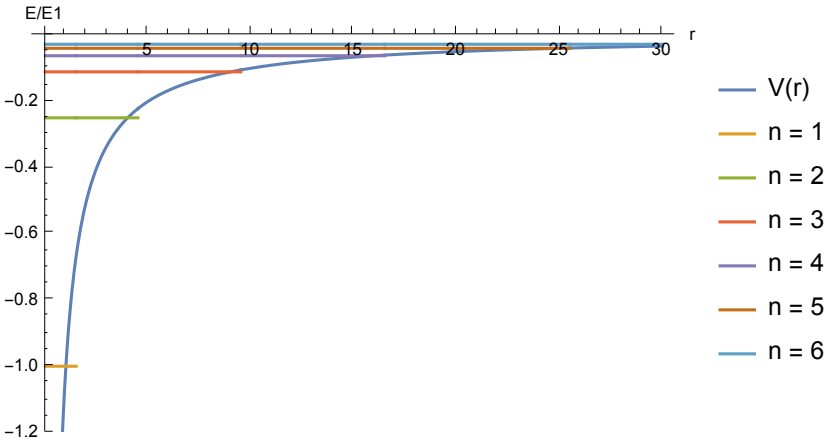
Out[•]=



3.A.2. El espectro.

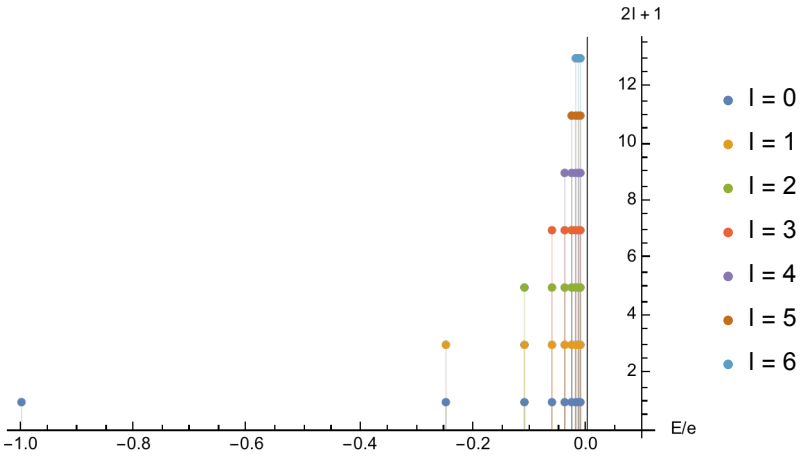
```
In[•]:= Plot[{-1 / r, If[r < 1 + 0.5, - 1], If[r < 4 + 0.5, - 1 / 4], If[r < 9 + 0.5, - 1 / 9],
          If[r < 16 + 0.5, - 1 / 16], If[r < 25 + 0.5, - 1 / 25], If[r < 36 + 0.5, - 1 / 36]},
         {r, 0, 30}, PlotRange → {-1.2, 0}, AxesLabel → {"r", "E/E1"},
         PlotLegends → Join[{"V(r)"}, Table["n = " <> ToString[n], {n, 6}]]]
```

Out[•]=




```
In[•]:= Show[
         ListPlot[Table[Table[{-1 / n^2, 2 * l + 1}, {n, 1 + l, 9}], {l, 0, 6}], Filling → Axis,
          PlotRange → All, AxesOrigin → {0.1, 0}, AxesLabel → {"E/e", "2l + 1"},
          PlotLegends → Table["l = " <> ToString[l], {l, 0, 6}]],
         Graphics[{Black, Line[{{0, 0}, {0, 14}}]}]]
```

Out[•]=



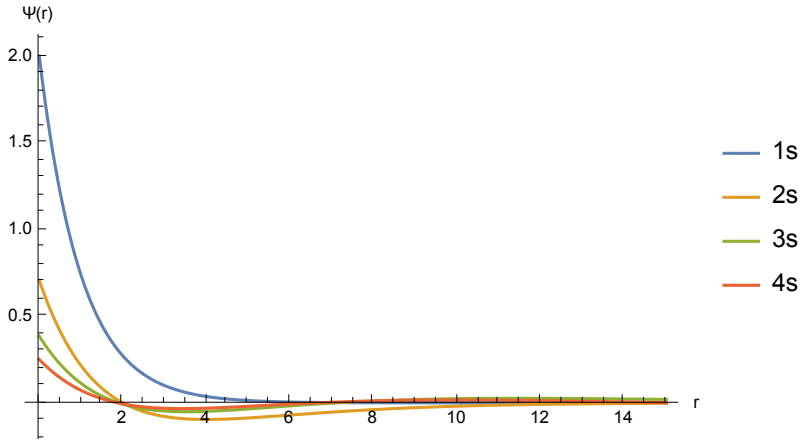
3.A.3. Las funciones de onda y las distribuciones radiales.

Las funciones.

Los orbitales tipo s.

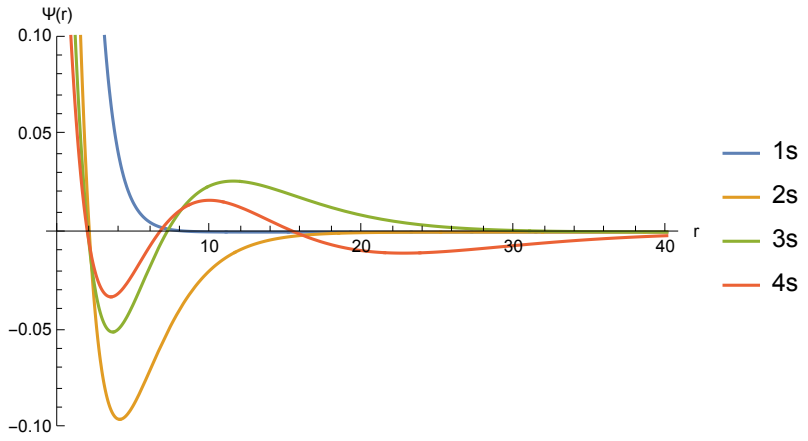
In[•]:=
```
Plot[{radhid[1, 0, r] * nohid[1, 0], radhid[2, 0, r] * nohid[2, 0],
  radhid[3, 0, r] * nohid[3, 0], radhid[4, 0, r] * nohid[4, 0]},
 {r, 0, 15}, PlotRange → All, PlotLegends → {"1s", "2s", "3s", "4s"},
 AxesLabel → {"r", "Ψ(r)"}]
```

Out[•]=



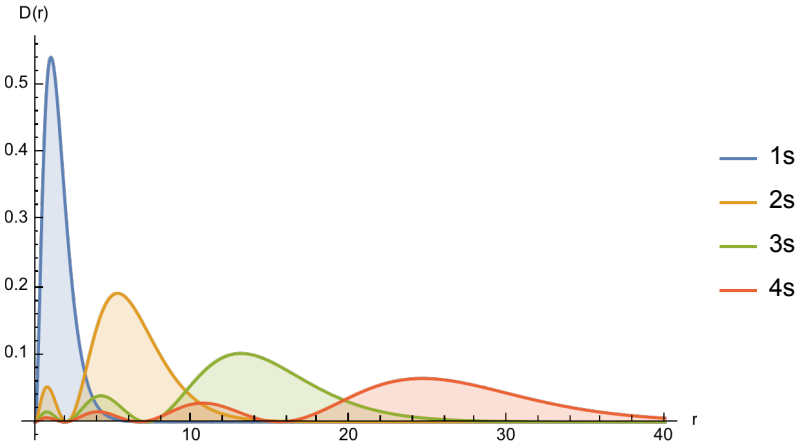
In[•]:=
```
Plot[{radhid[1, 0, r] * nohid[1, 0], radhid[2, 0, r] * nohid[2, 0],
  radhid[3, 0, r] * nohid[3, 0], radhid[4, 0, r] * nohid[4, 0]}, {r, 0, 40},
 PlotRange → {-0.1, 0.1}, PlotLegends → {"1s", "2s", "3s", "4s"},
 AxesLabel → {"r", "Ψ(r)"}]
```

Out[•]=



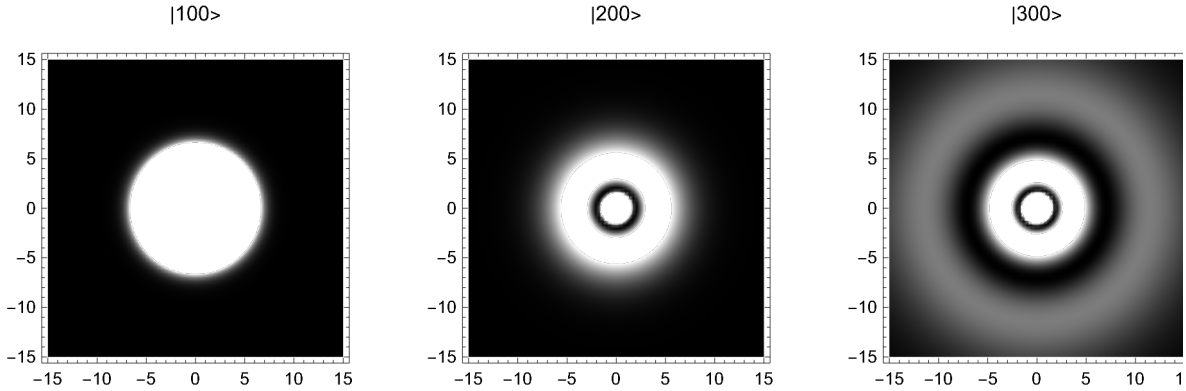
In[•]:=
```
Plot[{(radhid[1, 0, r] * r * nohid[1, 0]) ^ 2, (radhid[2, 0, r] * r * nohid[2, 0]) ^ 2,
  (radhid[3, 0, r] * r * nohid[3, 0]) ^ 2, (radhid[4, 0, r] * r * nohid[4, 0]) ^ 2},
 {r, 0, 40}, PlotRange → All, PlotLegends → {"1s", "2s", "3s", "4s"},
 AxesLabel → {"r", "D(r)"}, Filling → Axis]
```

Out[•]=



In[•]:=
```
GraphicsGrid[
 {{DensityPlot[(radhid[1, 0, Sqrt[x * x + z * z]] * nohid[1, 0] * SphericalHarmonicY[0,
        0, ArcCos[z / Sqrt[x * x + z * z]], 0]) ^ 2, {x, -15, 15}, {z, -15, 15},
   ColorFunction → GrayLevel, PlotPoints → 80, PlotLabel → "|100>"],
  DensityPlot[(radhid[2, 0, Sqrt[x * x + z * z]] * nohid[2, 0] *
      SphericalHarmonicY[0, 0, ArcCos[z / Sqrt[x * x + z * z]], 0]) ^ 2,
   {x, -15, 15}, {z, -15, 15}, ColorFunction → GrayLevel,
   PlotPoints → 80, PlotLabel → "|200>"],
  DensityPlot[(radhid[3, 0, Sqrt[x * x + z * z]] * nohid[3, 0] *
      SphericalHarmonicY[0, 0, ArcCos[z / Sqrt[x * x + z * z]], 0]) ^ 2,
   {x, -15, 15}, {z, -15, 15}, ColorFunction → GrayLevel,
   PlotPoints → 80, PlotLabel → "|300>"]}}]
```

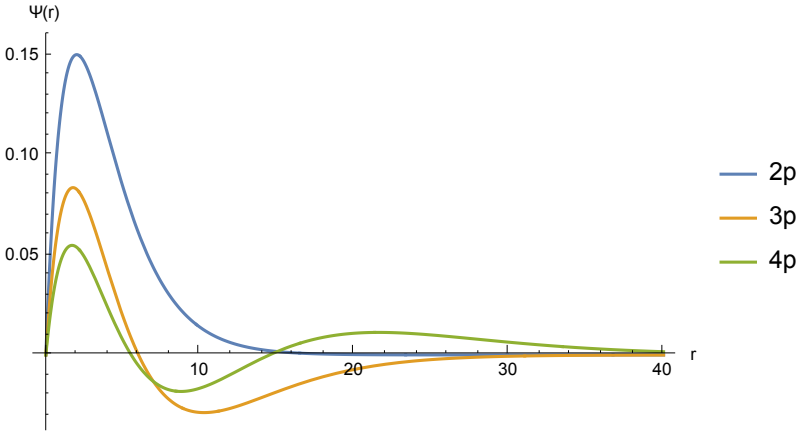
Out[•]=



Los orbitales tipo p.

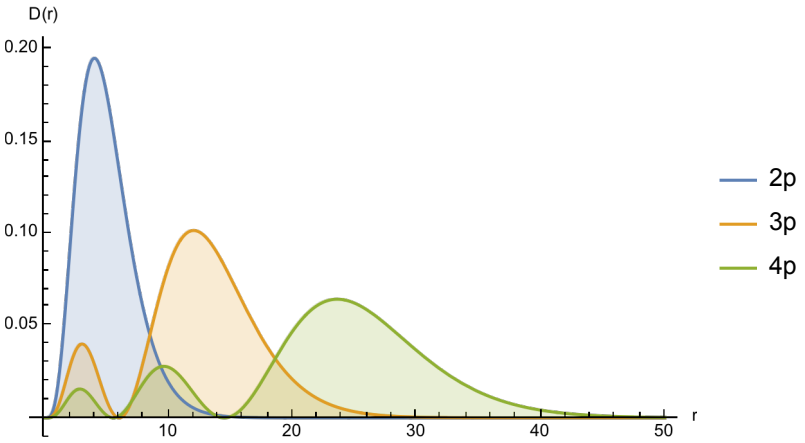
In[•]:=
```
Plot[{radhid[2, 1, r] * nohid[2, 1], radhid[3, 1, r] * nohid[3, 1],
  radhid[4, 1, r] * nohid[4, 1]}, {r, 0, 40}, PlotRange → All,
 PlotLegends → {"2p", "3p", "4p"}, AxesLabel → {"r", "Ψ(r)"}]
```

Out[•]=



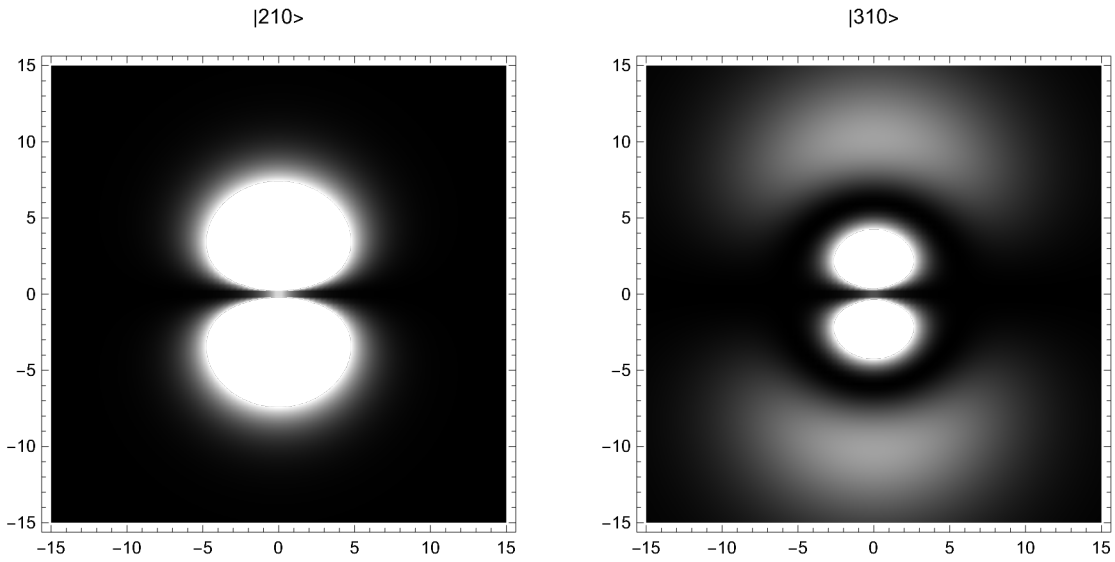
In[•]:=
```
Plot[{(radhid[2, 1, r] * r * nohid[2, 1]) ^ 2, (radhid[3, 1, r] * r * nohid[3, 1]) ^ 2,
  (radhid[4, 1, r] * r * nohid[4, 1]) ^ 2}, {r, 0, 50}, PlotRange → All,
 PlotLegends → {"2p", "3p", "4p"}, AxesLabel → {"r", "D(r)"}, Filling → Axis]
```

Out[•]=



In[•]:=
```
GraphicsGrid[
 {{DensityPlot[(radhid[2, 1, Sqrt[x * x + z * z]] * nohid[2, 1] * SphericalHarmonicY[1,
        0, ArcCos[z / Sqrt[x * x + z * z]], 0]) ^ 2, {x, -15, 15}, {z, -15, 15},
    ColorFunction → GrayLevel, PlotPoints → 80, PlotLabel → "|210>"],
   DensityPlot[(radhid[3, 1, Sqrt[x * x + z * z]] * nohid[3, 1] *
       SphericalHarmonicY[1, 0, ArcCos[z / Sqrt[x * x + z * z]], 0]) ^ 2,
    {x, -15, 15}, {z, -15, 15}, ColorFunction → GrayLevel,
    PlotPoints → 80, PlotLabel → "|310>"]}}]
```

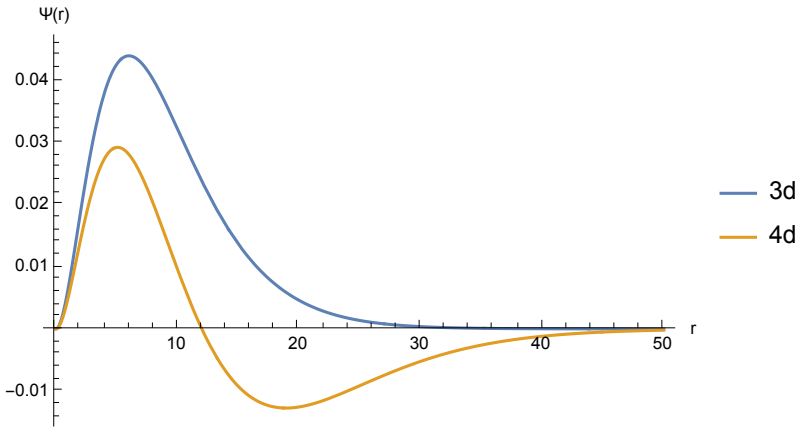
Out[•]=



Los orbitales tipo d.

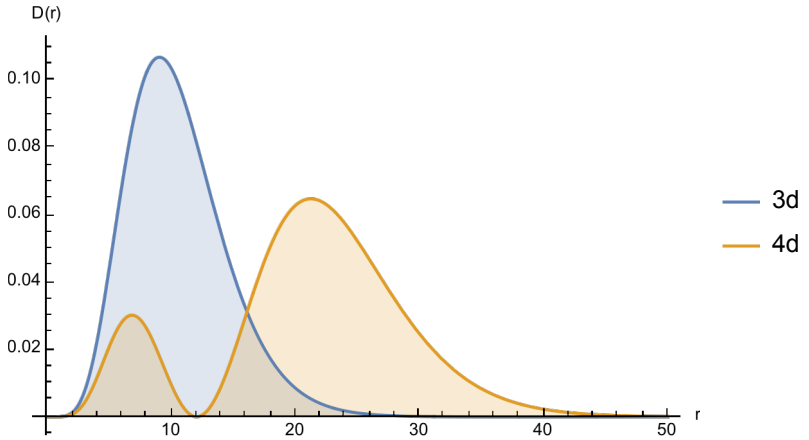
In[•]:=
```
Plot[{radhid[3, 2, r] * nohid[3, 2], radhid[4, 2, r] * nohid[4, 2]}, {r, 0, 50},
 PlotRange → All, PlotLegends → {"3d", "4d"}, AxesLabel → {"r", "Ψ(r)"}]
```

Out[•]=



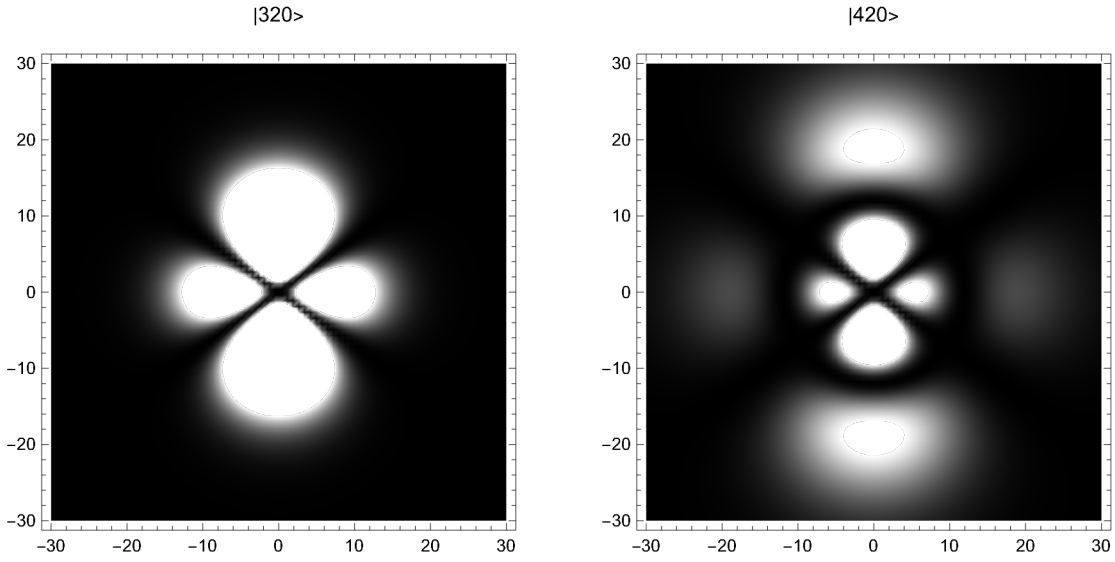
In[•]:=
```
Plot[{(radhid[3, 2, r] * r * nohid[3, 2]) ^ 2, (radhid[4, 2, r] * r * nohid[4, 2]) ^ 2},
 {r, 0, 50}, PlotRange → All, PlotLegends → {"3d", "4d"},
 AxesLabel → {"r", "D(r)"}, Filling → Axis]
```

Out[•]=



In[•]:=
```
GraphicsGrid[
 {{DensityPlot[(radhid[3, 2, Sqrt[x * x + z * z]] * nohid[3, 2] * SphericalHarmonicY[2,
        0, ArcCos[z / Sqrt[x * x + z * z]], 0]) ^ 2, {x, -30, 30}, {z, -30, 30},
    ColorFunction → GrayLevel, PlotPoints → 80, PlotLabel → "|320>"],
   DensityPlot[(radhid[4, 2, Sqrt[x * x + z * z]] * nohid[4, 2] *
       SphericalHarmonicY[2, 0, ArcCos[z / Sqrt[x * x + z * z]], 0]) ^ 2,
    {x, -30, 30}, {z, -30, 30}, ColorFunction → GrayLevel,
    PlotPoints → 80, PlotLabel → "|420>"]}}]
```

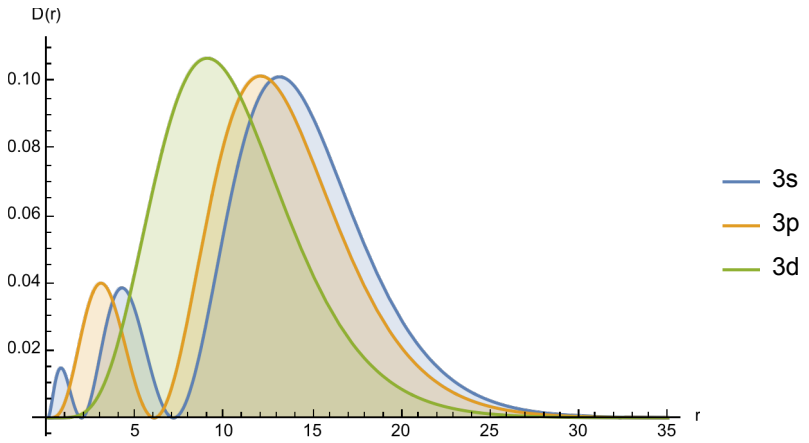
Out[•]=



Los orbitales de la capa n = 3.

In[•]:=
```
Plot[{(radhid[3, 0, r] * r * nohid[3, 0]) ^ 2, (radhid[3, 1, r] * r * nohid[3, 1]) ^ 2,
  (radhid[3, 2, r] * r * nohid[3, 2]) ^ 2}, {r, 0, 35}, PlotRange → All,
 PlotLegends → {"3s", "3p", "3d"}, AxesLabel → {"r", "D(r)"}, Filling → Axis]
```

Out[•]=



In[•]:=
```
NSolve[Simplify[D[(r * radhid[3, 0, r]) ^ 2, r] / r * Exp[2 * r / 3]], r]
```

Out[•]=
```
{{r → 0.740037}, {r → 1.90192}, {r → 4.18593}, {r → 7.09808}, {r → 13.074}}
```

In[•]:=
```
Print["Puntos críticos:"]
Table[{"l = " <> ToString[l],
    NSolve[D[(r * radhid[3, l, r]) ^ 2, r] / r ^ (2 * l + 1) * Exp[2 * r / 3] == 0, r]},
  {l, 0, 2}] // N // TableForm
```

```
Puntos críticos:
```

Out[•]//TableForm=

l = 0	r → 13.074
	r → 7.09808
	r → 4.18593
	r → 1.90192
	r → 0.740037
l = 1	r → 12.
	r → 6.
	r → 3.
l = 2	r → 9.

In[•]:=
```
Print["Nodos:"]
Table[{"l = " <> ToString[l], NSolve[radhid[3, l, r] / r ^ l * Exp[r / 3] == 0, r]},
  {l, 0, 2}] // N // TableForm
```

```
Nodos:
```

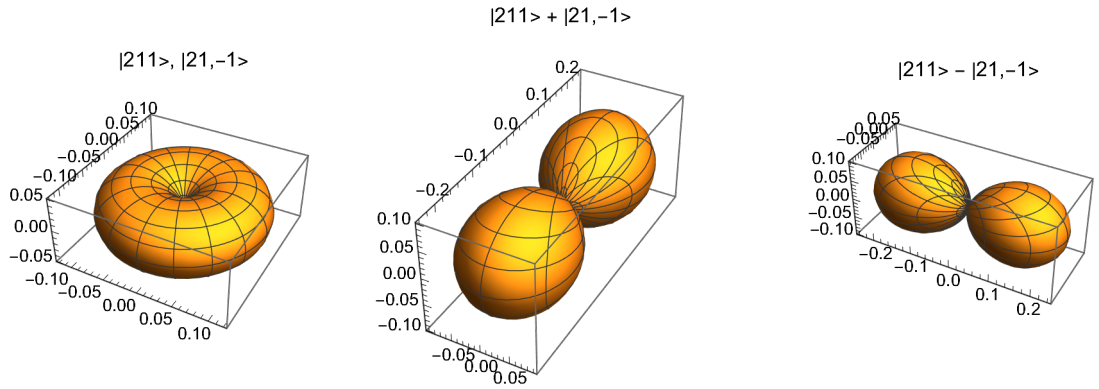
Out[•]//TableForm=

l = 0	r → 1.90192
	r → 7.09808
l = 1	r → 6.
l = 2	

3.A.4. Los orbitales reales.

In[•]:=
```
GraphicsGrid[
 {{SphericalPlot3D[(Abs[SphericalHarmonicY[1, 1, t, f]])^2, {t, 0, Pi},
    {f, 0, 2 * Pi}, PlotPoints → 50, PlotRange → All,
    PlotLabel → "|211>, |21,-1>"], SphericalPlot3D[
    (Abs[SphericalHarmonicY[1, 1, t, f] + SphericalHarmonicY[1, -1, t, f]])^2 / 2,
    {t, 0, Pi}, {f, 0, 2 * Pi}, PlotPoints → 50, PlotRange → All,
    PlotLabel → "|211> + |21,-1>"], SphericalPlot3D[
    (Abs[SphericalHarmonicY[1, 1, t, f] - SphericalHarmonicY[1, -1, t, f]])^2 / 2,
    {t, 0, Pi}, {f, 0, 2 * Pi}, PlotPoints → 50,
    PlotRange → All, PlotLabel → "|211> - |21,-1>"]}}]
```

Out[•]=



3.A.5. La absorción de la radiación.

Las integrales dipolares.

L = 0 <=> L = 1

In[•]:=
```
TableForm[Table[nohid[p, 1] * nohid[n, 0] *
    NIntegrate[radhid[p, 1, t] * radhid[n, 0, t] * t^3, {t, 0, Infinity}],
  {n, 1, 5}, {p, 2, 6}], TableHeadings →
  {Table["n=" <> ToString[n], {n, 1, 5}], Table["p=" <> ToString[p], {p, 2, 6}]}]
```

Out[•]//TableForm=

	p=2	p=3	p=4	p=5	p=6
n=1	1.29027	0.516689	0.304584	0.208704	0.155135
n=2	−5.19615	3.06482	1.28228	0.773952	0.540367
n=3	0.938404	−12.7279	5.46934	2.25958	1.36022
n=4	0.382301	2.44353	−23.2379	8.51783	3.4545
n=5	0.228028	0.96961	4.60028	−36.7423	12.2139

L = 1 <=> L = 2

```
In[•]:= TableForm[Table[nohid[p, 2] * nohid[n, 1] *
     NIntegrate[radhid[p, 2, t] * radhid[n, 1, t] * t^3, {t, 0, Infinity}],
    {n, 2, 6}, {p, 3, 7}], TableHeadings →
    {Table["n=" <> ToString[n], {n, 2, 6}], Table["p=" <> ToString[p], {p, 3, 7}]}]
```

Out[•]//TableForm=

	p=3	p=4	p=5	p=6	p=7
n=2	4.74799	1.7097	0.975087	0.661811	0.491626
n=3	−10.0623	7.56541	2.96832	1.74108	1.19966
n=4	1.30225	−20.7846	11.0389	4.38646	2.58589
n=5	0.482798	3.04532	−34.3693	15.1655	6.00466
n=6	0.275288	1.1229	5.42698	−50.9117	19.9438

L = 2 <= > L = 3

```
In[•]:= TableForm[Table[nohid[p, 3] * nohid[n, 2] *
     NIntegrate[radhid[p, 3, t] * radhid[n, 2, t] * t^3, {t, 0, Infinity}],
    {n, 3, 7}, {p, 4, 8}], TableHeadings →
    {Table["n=" <> ToString[n], {n, 3, 7}], Table["p=" <> ToString[p], {p, 4, 8}]}]
```

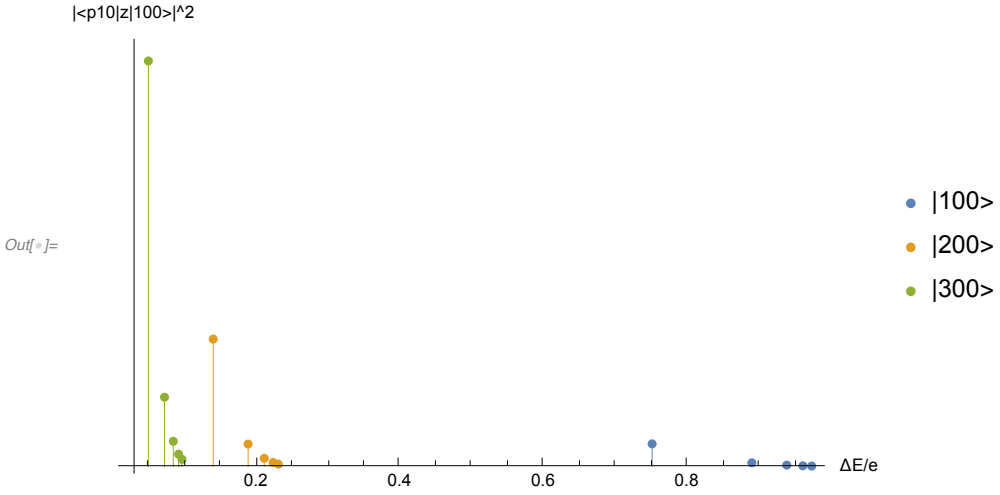
Out[•]//TableForm=

	p=4	p=5	p=6	p=7	p=8
n=3	10.2303	3.31868	1.79818	1.1876	0.868926
n=4	−15.8745	14.0653	5.17746	2.92948	1.97565
n=5	1.66131	−30.	18.585	7.08649	4.07168
n=6	0.564907	3.65113	−46.7654	23.7722	9.15615
n=7	0.306372	1.25838	6.26674	−66.4078	29.6196

El espectro de absorción.

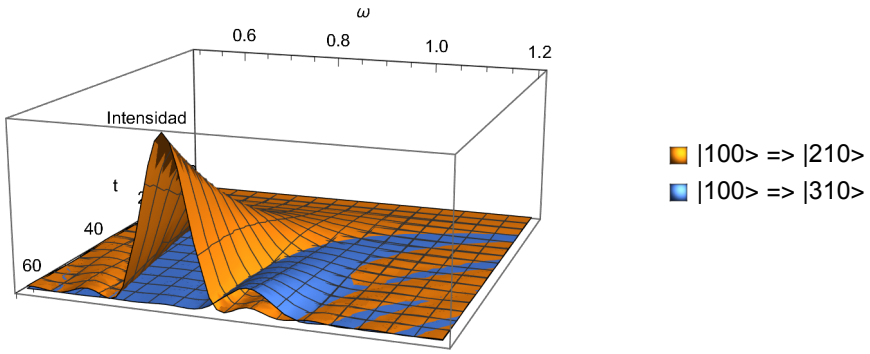
In[ ]:=
```
temp = Table[{1 - 1 / p^2, (nohid[p, 1] * nohid[1, 0] * NIntegrate[
          radhid[p, 1, t] * radhid[1, 0, t] * t^3, {t, 0, Infinity}])^2}, {p, 2, 6}];
temp = Append[{temp},
   Table[{1 / 4 - 1 / p^2, (nohid[p, 1] * nohid[2, 0] * NIntegrate[radhid[p, 1, t] *
          radhid[2, 0, t] * t^3, {t, 0, Infinity}])^2}, {p, 3, 7}]];
temp = Append[temp,
   Table[{1 / 9 - 1 / p^2, (nohid[p, 1] * nohid[3, 0] * NIntegrate[radhid[p, 1, t] *
          radhid[3, 0, t] * t^3, {t, 0, Infinity}])^2}, {p, 4, 8}]];
ListPlot[temp, Filling → Axis, FillingStyle → Opacity[1.0],
 AxesLabel → {"ΔE/e", "|<p10|z|100>|^2"}, Ticks → {True, False},
 PlotRange → All, PlotLegends → {"|100>", "|200>", "|300>"}]
```

Out[ ]=



In[•]:=
```
tempw = 1 - 1 / 4;
temp = (nohid[2, 1] * nohid[1, 0] *
      NIntegrate[radhid[1, 0, t] * radhid[2, 1, t] * t^3, {t, 0, Infinity}])^2;
tempv = 1 - 1 / 9;
tempi = (nohid[3, 1] * nohid[1, 0] *
      NIntegrate[radhid[1, 0, t] * radhid[3, 1, t] * t^3, {t, 0, Infinity}])^2;
Plot3D[{temp * (Sin[(w - tempw) * t / 2] / (w - tempw))^2,
  tempi * (Sin[(w - tempv) * t / 2] / (w - tempv))^2}, {t, 0, 64},
 {w, 0.5, 1.2}, PlotRange → All, AxesLabel → {"t", "ω", "Intensidad"},
 Ticks → {True, True, False}, PlotLegends → {"|100> => |210>", "|100> => |310>"}]
```

Out[•]=

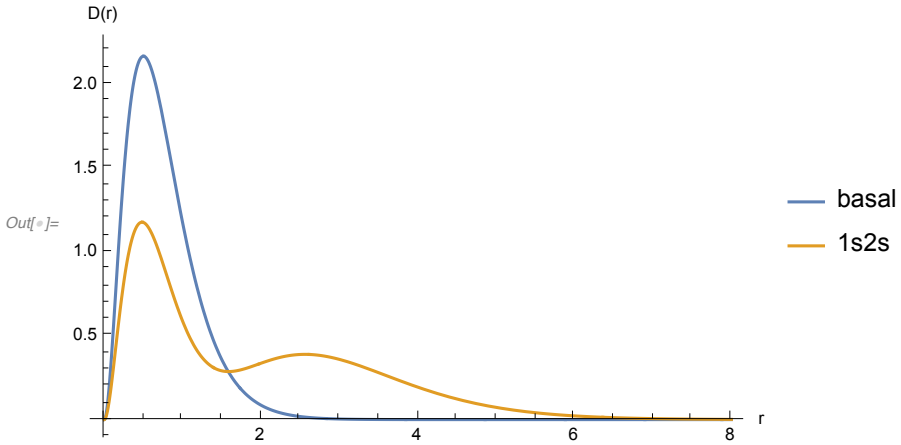


3.B. El átomo de helio.

3.B.1. La función de onda aproximada con orbitales hidrogenoides.

```
In[•]:= Plot[{2 * (nohid[1, 0] * radhid[1, 0, 2 * r]) ^ 2 * 8 * r * r,
    ((nohid[1, 0] * radhid[1, 0, 2 * r]) ^ 2 + (nohid[2, 0] * radhid[2, 0, 2 * r]) ^ 2) *
     8 * r * r}, {r, 0, 8}, AxesLabel → {"r", "D(r)"},
  PlotRange → All, PlotLegends → {"basal", "1s2s"}]
```

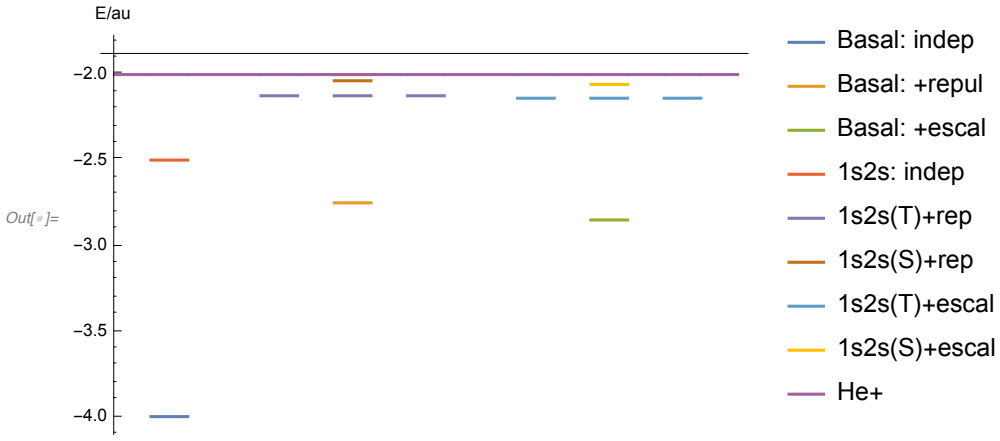
Out[•]=



3.B.2. La repulsión en forma perturbativa.

```
In[•]:= Plot[{If[x > 1 && x < 2, -4], If[x > 6 && x < 7, -2.75],
    If[x > 13 && x < 14, -2.85], If[x > 1 && x < 2, -2.5],
    If[x > 4 && x < 5 || x > 6 && x < 7 || x > 8 && x < 9, -2.5 + 34 / 81 - 32 / 729],
    If[x > 6 && x < 7, -2.5 + 34 / 81 + 32 / 729],
    If[x > 11 && x < 12 || x > 13 && x < 14 || x > 15 && x < 16, -2.1383],
    If[x > 13 && x < 14, -2.0578], -2}, {x, 0, 17},
  PlotLegends → {"Basal: indep", "Basal: +repul", "Basal: +escal", "1s2s: indep",
    "1s2s(T)+rep", "1s2s(S)+rep", "1s2s(T)+escal", "1s2s(S)+escal", "He+"},
  Ticks → {False, True}, PlotRange → All, AxesLabel → {"", "E/au"}]
```

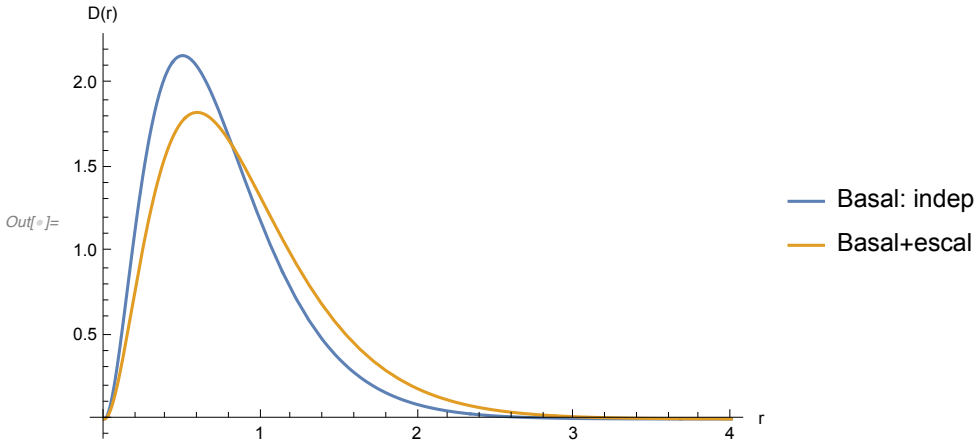
Out[•]=



3.B.3. Las funciones de onda escaladas.

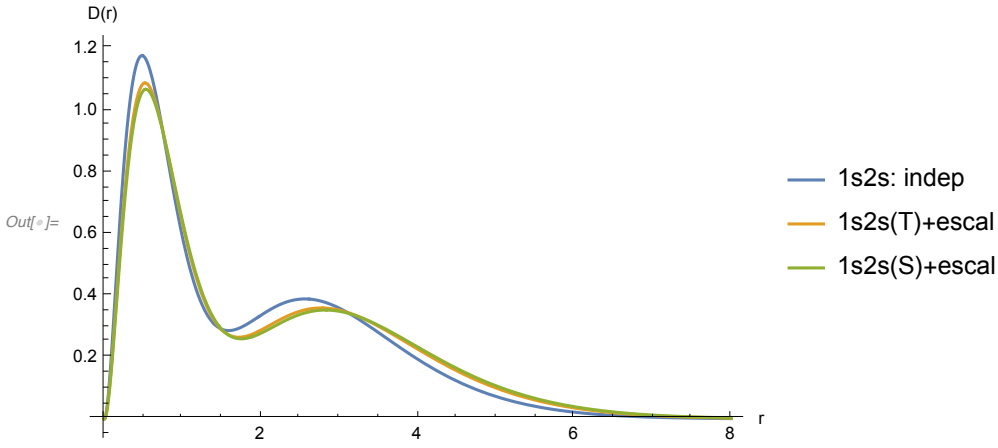
In[•]:=
```
Plot[{2 * (nohid[1, 0] * radhid[1, 0, 2 * r]) ^ 2 * 8 * r * r,
  2 * (nohid[1, 0] * radhid[1, 0, 2 * r * 27 / 32]) ^ 2 * 8 * (27 / 32) ^ 3 * r * r},
 {r, 0, 4}, AxesLabel → {"r", "D(r)"}, PlotRange → All,
 PlotLegends → {"Basal: indep", "Basal+escal"}]
```

Out[•]=



In[•]:=
```
Plot[{ ((nohid[1, 0] * radhid[1, 0, 2 * r]) ^ 2 + (nohid[2, 0] * radhid[2, 0, 2 * r]) ^ 2) *
   8 * r * r, ((nohid[1, 0] * radhid[1, 0, 2 * r * 0.9248]) ^ 2 +
     (nohid[2, 0] * radhid[2, 0, 2 * r * 0.9248]) ^ 2) * 8 * (0.9248) ^ 3 * r * r,
  ((nohid[1, 0] * radhid[1, 0, 2 * r * 0.9073]) ^ 2 +
     (nohid[2, 0] * radhid[2, 0, 2 * r * 0.9073]) ^ 2) * 8 * (0.9073) ^ 3 * r * r},
 {r, 0, 8}, AxesLabel → {"r", "D(r)"}, PlotRange → All,
 PlotLegends → {"1s2s: indep", "1s2s(T)+escal", "1s2s(S)+escal"}]
```

Out[•]=



3.C. Los átomos polielectrónicos.

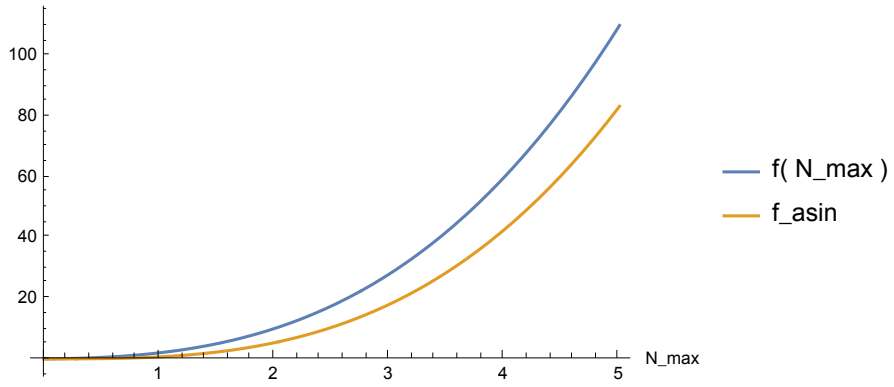
3.C.1. El modelo de las partículas independientes.

Las funciones.

Las tendencias.

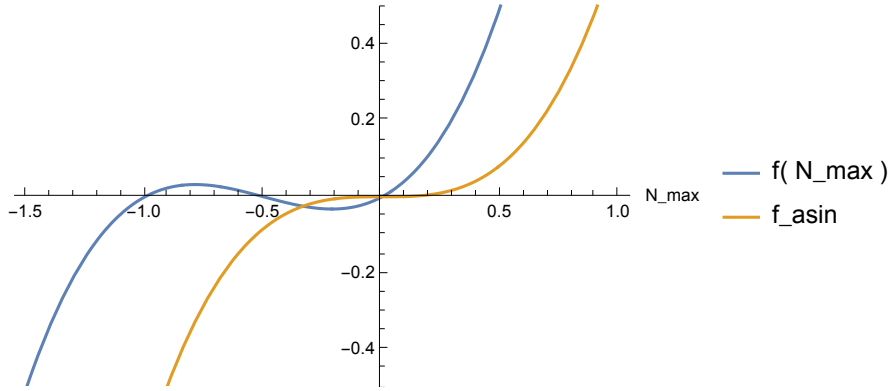
```
In[•]:= Plot[{x * (x + 1) * (2 * x + 1) / 3, 2 * x * x * x / 3}, {x, 0, 5},
         AxesLabel → {"N_max"}, PlotLegends → {"f( N_max )", "f_asin"}]
```

Out[•]=



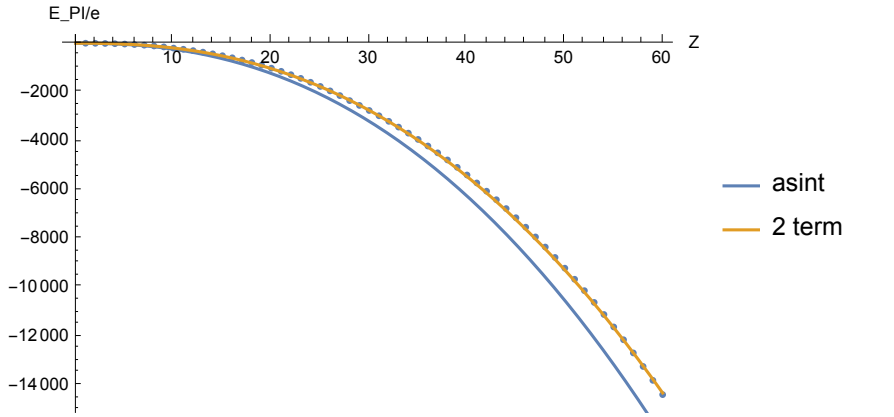

```
In[•]:= Plot[{x * (x + 1) * (2 * x + 1) / 3, 2 * x * x * x / 3},
         {x, -1.5, 1.0}, AxesLabel → {"N_max"},
         PlotLegends → {"f( N_max )", "f_asin"}, PlotRange → {-0.5, 0.5}]
```

Out[•]=



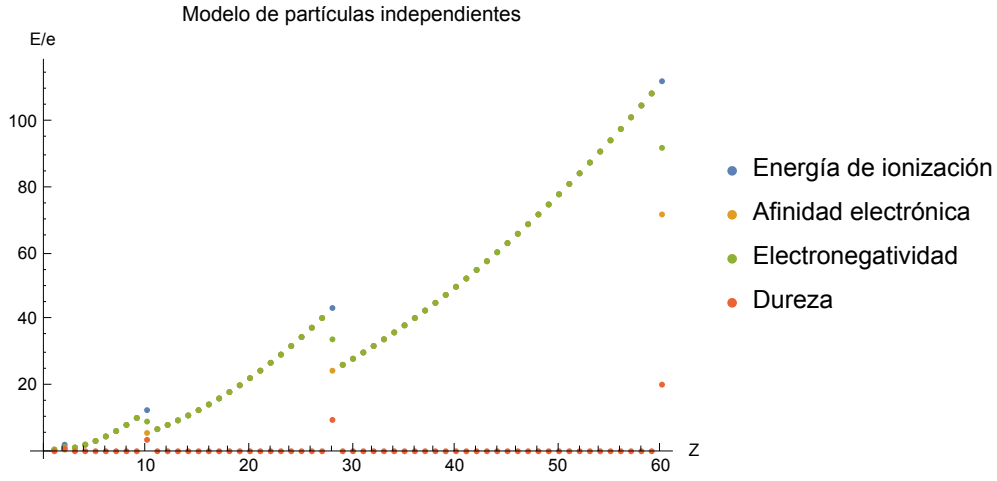

```
In[•]:= temp = Table[N[epi[n, n]], {n, 1, 60}];
        Show[ListPlot[temp, AxesLabel → {"Z", "E_PI/e"}],
         Plot[{-x * x * (3 * x / 2) ^ (1 / 3), -x * x * ((3 * x / 2) ^ (1 / 3) - 1 / 2)},
          {x, 0, 60}, PlotLegends → {"asint", "2 term"}]]
```

Out[•]=



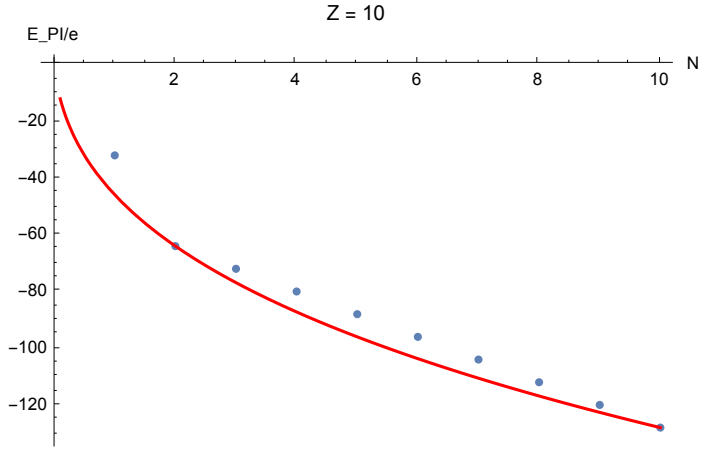
In[•]:=
```
temp = {Table[N[epi[n - 1, n] - epi[n, n]], {n, 1, 60}],
    Table[N[epi[n, n] - epi[n + 1, n]], {n, 1, 60}],
    Table[N[-epi[n + 1, n] + epi[n - 1, n]] / 2, {n, 1, 60}],
    Table[N[epi[n + 1, n] - 2 * epi[n, n] + epi[n - 1, n]] / 2, {n, 1, 60}]};
ListPlot[temp, AxesLabel → {"Z", "E/e"},
 PlotLabel → "Modelo de partículas independientes",
 PlotLegends → {"Energía de ionización",
   "Afinidad electrónica", "Electronegatividad", "Dureza"}]
```

Out[•]=



In[•]:=
```
temp = Table[N[epi[n, 8]], {n, 1, 10}];
Show[ListPlot[temp, AxesLabel → {"N", "E_PI/e"}, PlotLabel → "Z = 10"],
 Plot[-64 * ((3 * x / 2) ^ (1 / 3) - 1 / 2 + 1 / 12 * (2 / (3 * x)) ^ (1 / 3)),
  {x, 0.1, 10}, PlotStyle → Red]]
```

Out[•]=



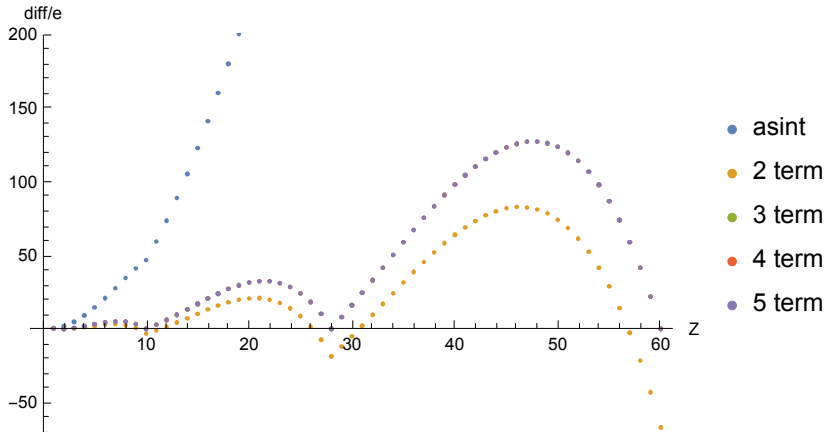
El análisis del modelo polinomial.

In[•]:=
```
temp =
  Normal[Series[((1 + Sqrt[1 - a]) / 2) ^ (1 / 3), {a, 0, 5}]] /. a → 4 * (w * w / 12) ^ 3;
Expand[temp - w / 2 + (Normal[Series[(2 * (1 - Sqrt[1 - a]) / a) ^ (1 / 3), {a, 0, 5}]] /.
      a → 4 * (w * w / 12) ^ 3) * w * w / 12]
```

Out[•]=
$$1 - \frac{w}{2} + \frac{w^2}{12} - \frac{w^6}{5184} + \frac{w^8}{62\,208} - \frac{w^{12}}{6\,718\,464} + \frac{5\,w^{14}}{322\,486\,272} - \frac{77\,w^{18}}{417\,942\,208\,512} + \frac{13\,w^{20}}{626\,913\,312\,768} - \frac{595\,w^{24}}{2\,166\,612\,408\,926\,208} + \frac{209\,w^{26}}{6\,499\,837\,226\,778\,624} - \frac{5083\,w^{30}}{11\,231\,718\,727\,873\,462\,272} + \frac{7315\,w^{32}}{134\,780\,624\,734\,481\,547\,264}$$

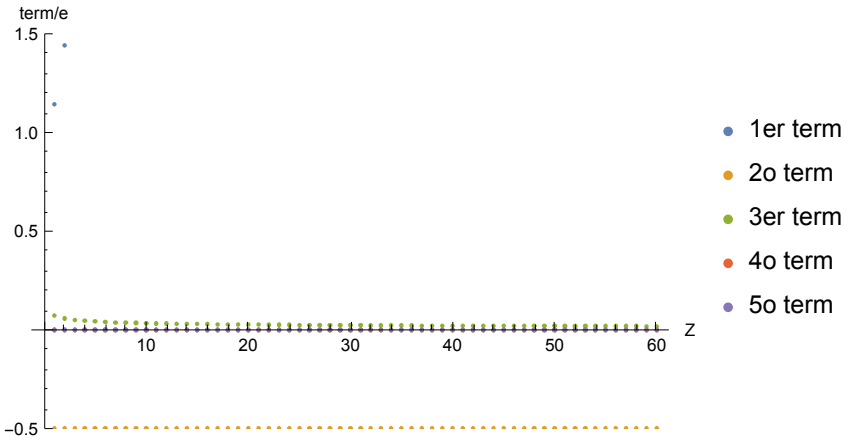
In[•]:=
```
temp = {Table[epi[n, n] + n * n * (3 * n / 2) ^ (1 / 3), {n, 1, 60}],
    Table[epi[n, n] + n * n * ((3 * n / 2) ^ (1 / 3) - 1 / 2), {n, 1, 60}], Table[epi[n, n] +
      n * n * ((3 * n / 2) ^ (1 / 3) - 1 / 2 + 1 / 12 * (2 / (3 * n)) ^ (1 / 3)), {n, 1, 60}],
    Table[epi[n, n] + n * n * ((3 * n / 2) ^ (1 / 3) - 1 / 2 + 1 / 12 * (2 / (3 * n)) ^ (1 / 3) -
        1 / (2 ^ 6 * 3 ^ 4) * (2 / (3 * n)) ^ (5 / 3)), {n, 1, 60}], Table[epi[n, n] +
      n * n * ((3 * n / 2) ^ (1 / 3) - 1 / 2 + 1 / 12 * (2 / (3 * n)) ^ (1 / 3) - 1 / (2 ^ 6 * 3 ^ 4) *
        (2 / (3 * n)) ^ (5 / 3) + 1 / (2 ^ 8 * 3 ^ 5) * (2 / (3 * n)) ^ (7 / 3)), {n, 1, 60}]};
ListPlot[temp, AxesLabel → {"Z", "diff/e"}, PlotRange → {-70, 200},
 PlotLegends → {"asint", "2 term", "3 term", "4 term", "5 term"}]
```

Out[•]=



```
In[•]:= temp = {Table[(3 * n / 2) ^ (1 / 3), {n, 1, 60}],
    Table[-1 / 2, {n, 1, 60}], Table[1 / 12 * (2 / (3 * n)) ^ (1 / 3), {n, 1, 60}],
    Table[-1 / (2 ^ 6 * 3 ^ 4) * (2 / (3 * n)) ^ (5 / 3), {n, 1, 60}],
    Table[1 / (2 ^ 8 * 3 ^ 5) * (2 / (3 * n)) ^ (7 / 3), {n, 1, 60}]};
  ListPlot[temp, AxesLabel → {"Z", "term/e"}, PlotRange → {-0.5, 1.5},
   PlotLegends → {"1er term", "2o term", "3er term", "4o term", "5o term"}]
```

Out[•]=



3.C.2. Las integrales bielectrónicas con orbitales hidrogenoides tipo s.

Las funciones hidrogenoides.

Las fórmulas de integración.

Algunos ejemplos.

```
In[•]:= n1s = {1, 0, Z}; n2s = {2, 0, Z}; n3s = {3, 0, Z};
```

1s 1s

```
In[•]:= {jhs = Js[n1s, n1s], khs = Ks[n1s, n1s], khs / jhs}
```

Out[•]= $\left\{\frac{5\,Z}{8}, \frac{5\,Z}{8}, 1\right\}$

1s 2s

```
In[•]:= {jhs = Js[n1s, n2s], khs = Ks[n1s, n2s], khs / jhs}
```

Out[•]= $\left\{\frac{17\,Z}{81}, \frac{16\,Z}{729}, \frac{16}{153}\right\}$

```
In[•]:= IB4s[n1s, n1s, n1s, n2s]
```

Out[•]= $\frac{4096\,\sqrt{2}\,Z}{64\,827}$

```
In[•]:= IB4s[n1s, n2s, n2s, n2s]
```

Out[•]= $\frac{512\,\sqrt{2}\,Z}{84\,375}$

2s 2s

```
In[•]:= {jhs = Js[n2s, n2s], khs = Ks[n2s, n2s], khs / jhs}
```

$$\text{Out}[\bullet]= \left\{\frac{77\,Z}{512}, \frac{77\,Z}{512}, 1\right\}$$

1s 3s

```
In[•]:= {jhs = Js[n3s, n1s], khs = Ks[n3s, n1s], khs / jhs}
```

$$\text{Out}[\bullet]= \left\{\frac{815\,Z}{8192}, \frac{189\,Z}{32\,768}, \frac{189}{3260}\right\}$$

2s 3s

```
In[•]:= {jhs = Js[n3s, n2s], khs = Ks[n3s, n2s], khs / jhs}
```

$$\text{Out}[\bullet]= \left\{\frac{32\,857\,Z}{390\,625}, \frac{73\,008\,Z}{9\,765\,625}, \frac{73\,008}{821\,425}\right\}$$

3s 3s

```
In[•]:= {jhs = Js[n3s, n3s], khs = Ks[n3s, n3s], khs / jhs}
```

$$\text{Out}[\bullet]= \left\{\frac{17\,Z}{256}, \frac{17\,Z}{256}, 1\right\}$$

3.C.3. La repulsión electrónica en forma perturbativa

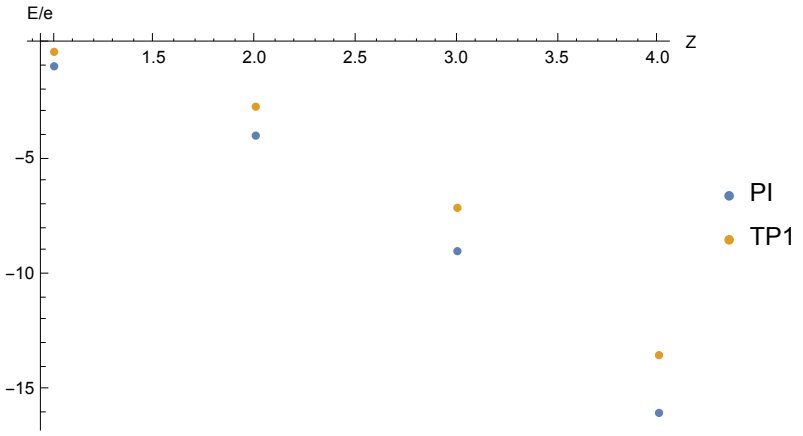
Las funciones.

N = 2

```
In[•]:= tempj1 = Js[n1s, n1s];
```

```
In[•]:= temp = {Table[{z, 2 * ehid[1, z]}, {z, 1, 4}],
    Table[{z, 2 * ehid[1, z] + tempj1 /. Z → z}, {z, 1, 4}]};
ListPlot[temp, AxesLabel → {"Z", "E/e"}, PlotLegends → {"PI", "TP1"}]
```

Out[•]=

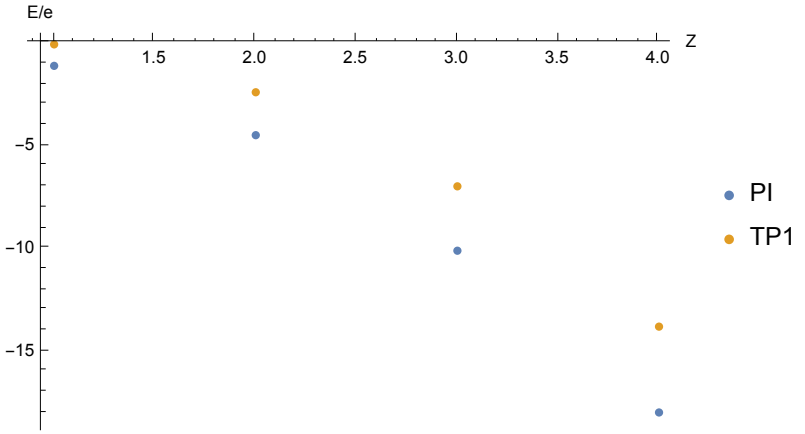


N = 3

```
In[•]:= tempj1 = Js[n1s, n1s];
tempj2 = Js[n1s, n2s];
```

In[•]:=
```
temp = {Table[{z, 2 * ehid[1, z] + ehid[2, z]}, {z, 1, 4}],
   Table[{z, 2 * ehid[1, z] + ehid[2, z] + (tempj1 + 2 * tempj2) /. Z → z}, {z, 1, 4}]};
ListPlot[temp, AxesLabel → {"Z", "E/e"}, PlotLegends → {"PI", "TP1"}]
```

Out[•]=

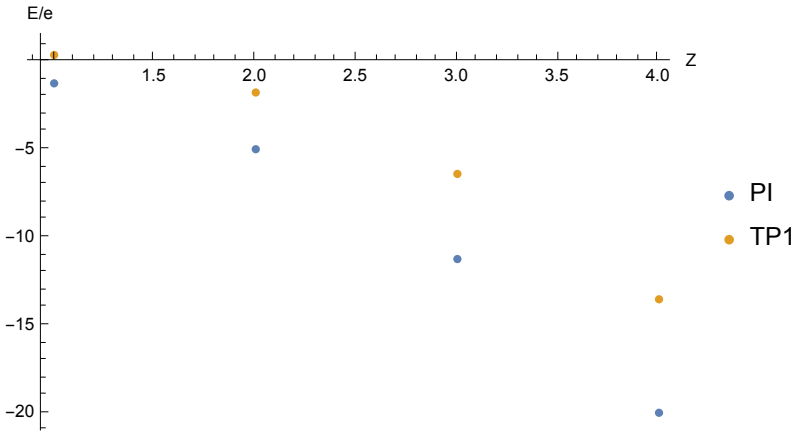


N = 4

In[•]:=
```
tempj1 = Js[n1s, n1s];
tempj2 = Js[n1s, n2s];
tempj3 = Js[n2s, n2s];
```

In[•]:=
```
temp = {Table[{z, 2 * ehid[1, z] + 2 * ehid[2, z]}, {z, 1, 4}],
   Table[{z, 2 * ehid[1, z] + 2 * ehid[2, z] + (tempj1 + 4 * tempj2 + tempj3) /. Z → z},
    {z, 1, 4}]};
ListPlot[temp, AxesLabel → {"Z", "E/e"}, PlotLegends → {"PI", "TP1"}]
```

Out[•]=

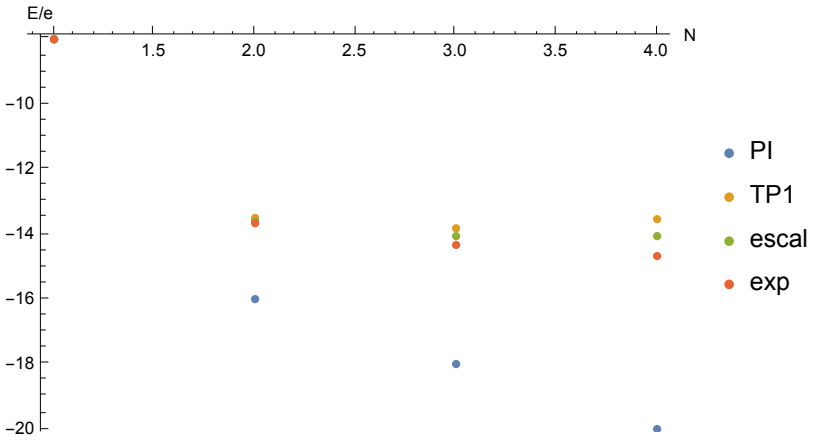


Z = 4

In[•]:=
```
tempj1 = Js[n1s, n1s];
tempj2 = Js[n1s, n2s];
tempj3 = Js[n2s, n2s];
```

```
In[•]:= temp = {{{1, ehid[1, 4]}, {2, 2 * ehid[1, 4]},
      {3, 2 * ehid[1, 4] + ehid[2, 4]}, {4, 2 * (ehid[1, 4] + ehid[2, 4])}},
     {{1, ehid[1, 4]}, {2, 2 * ehid[1, 4] + (tempj1) /. Z → 4},
      {3, 2 * ehid[1, 4] + ehid[2, 4] + (tempj1 + 2 * tempj2) /. Z → 4},
      {4, 2 * (ehid[1, 4] + ehid[2, 4]) + (tempj1 + 4 * tempj2 + tempj3) /. Z → 4}},
     {{1, ehid[1, 4]}, {2, (2 * ehid[1, 4]) / 4 *
        (2 + ((tempj1) /. Z → 4) / (2 * ehid[1, 4]))^2},
      {3, (2 * ehid[1, 4] + ehid[2, 4]) / 4 *
        (2 + ((tempj1 + 2 * tempj2) /. Z → 4) / (2 * ehid[1, 4] + ehid[2, 4]))^2},
      {4, (2 * (ehid[1, 4] + ehid[2, 4])) / 4 *
        (2 + ((tempj1 + 4 * tempj2 + tempj3) /. Z → 4) / (2 * (ehid[1, 4] + ehid[2, 4])))^
         2}}, {{4, -14.676}, {3, -14.334}, {2, -13.664}, {1, -8.005}}};
ListPlot[temp, AxesLabel → {"N", "E/e"},
 PlotLegends → {"PI", "TP1", "escal", "exp"}, PlotRange → {-20.1, -7.9}]
```

Out[•]=



3.C.4. El método de Hartree.

Un cálculo para dos electrones en el estado basal.

Se usan orbitales tipo Slater (STO).

Las funciones.

2 funciones, exponente atómico.

```
In[•]:= tempp1 = Plot[8 * Pi * r * r / 2 * fchi[0, 2, r]^2,
     {r, 0, 5}, PlotRange → All, AxesLabel → {"r", "D(r)"}];
```

```
In[•]:= n = 1;
z = 2;
a = z;
U = {1, 0};
```

```
In[•]:= Hydro = HM[n, z, a];
        Biele = CM[n];
        Trasl = SM[n, a];
        Vee = JM[n, U, a, Biele];
        {N[Ene[n, U, z, a, Hydro, Vee]], U}
Out[•]= {-2.75, {1, 0}}

In[•]:= For[i = 0, i < 10, i++ ,
         M = Hydro + Vee - x * Trasl;
         X = NSolve[Det[M] == 0, x];
         V = NullSpace[M /. X[[1]]];
         U = V[[1]] / V[[1]][[1]];
         Vee = JM[n, U, a, Biele];
         Print[{Ene[n, U, z, a, Hydro, Vee], U}]
        ]
        {-2.83407, {1., 0.159742}}
        {-2.83749, {1., 0.118985}}
        {-2.83764, {1., 0.126782}}
        {-2.83764, {1., 0.125184}}
        {-2.83764, {1., 0.125507}}
        {-2.83764, {1., 0.125441}}
        {-2.83764, {1., 0.125455}}
        {-2.83764, {1., 0.125452}}
        {-2.83764, {1., 0.125453}}
        {-2.83764, {1., 0.125452}}

In[•]:= Print[{Ene[n, U, z, a, Hydro, Vee], U}]
        {-2.83764, {1., 0.125452}}

In[•]:= tempp2 = Plot[8 * Pi * r * r / CO[n, U] * (U.Table[fchi[i, a, r], {i, 0, n}]) ^ 2,
            {r, 0, 5}, PlotRange → All, AxesLabel → {"r", "D(r)"}];
```

3 funciones, exponente atómico.

```
In[•]:= n = 2;
        z = 2;
        a = z;
        U = {1, 0, 0};

In[•]:= Hydro = HM[n, z, a];
        Biele = CM[n];
        Trasl = SM[n, a];
        Vee = JM[n, U, a, Biele];
        {N[Ene[n, U, z, a, Hydro, Vee]], U}
Out[•]= {-2.75, {1, 0, 0}}
```

```
For[i = 0, i < 10, i++ ,
 M = Hydro + Vee - x * Trasl;
 X = NSolve[Det[M] == 0, x];
 V = NullSpace[M /. X[[1]]];
 U = V[[1]] / V[[1]][[1]];
 Vee = JM[n, U, a, Biele];
 Print[{Ene[n, U, z, a, Hydro, Vee], U}]
]
```

```
Print[{Ene[n, U, z, a, Hydro, Vee], U}]
```

```
{-2.86146, {1., -0.0020931, 0.0708201}}
```

```
tempp3 = Plot[8 * Pi * r * r / CO[n, U] * (U.Table[fchi[i, a, r], {i, 0, n}]) ^2,
    {r, 0, 5}, PlotRange → All, AxesLabel → {"r", "D(r)"}];
```

4 funciones, exponente atómico.

5 funciones, exponente atómico.

6 funciones, exponente atómico.

2 funciones, exponente optimizado.

```
tempp1 = Plot[8 * Pi * r * r / 2 * fchi[0, 27 / 16, r] ^2,
    {r, 0, 5}, PlotRange → All, AxesLabel → {"r", "D(r)"}];
```

```
n = 1;
z = 2;
a = z - 5 / 16;
U = {1, 0};
```

```
Hydro = HM[n, z, a];
Biele = CM[n];
Trasl = SM[n, a];
Vee = JM[n, U, a, Biele];
{N[Ene[n, U, z, a, Hydro, Vee]], U}
```

Out[•]= {-2.84766, {1, 0}}

```
For[i = 0, i < 10, i++ ,
 M = Hydro + Vee - x * Trasl;
 X = NSolve[Det[M] == 0, x];
 V = NullSpace[M /. X[[1]]];
 U = V[[1]] / V[[1]][[1]];
 Vee = JM[n, U, a, Biele];
 Print[{Ene[n, U, z, a, Hydro, Vee], U}]
]
```

```
Print[{Ene[n, U, z, a, Hydro, Vee], U}]
```

```
{-2.84766, {1., 0.}}
```

```
In[•]:= tempp2 = Plot[8 * Pi * r * r / CO[n, U] * (U.Table[fchi[i, a, r], {i, 0, n}]) ^ 2,
          {r, 0, 5}, PlotRange → All, AxesLabel → {"r", "D(r)"}];
```

3 funciones, exponente optimizado.

4 funciones, exponente optimizado.

5 funciones, exponente optimizado.

6 funciones, exponente optimizado.

El resumen de los resultados.

```
In[•]:= temp = {{{1, -2.75}, {2, -2.83764104022273}, {3, -2.8614608110058573 },
           {4, -2.861579277960568}, {5, -2.861679425065577}},
          {{1, -2.84765625}, {2, -2.84765625}, {3, -2.8606340475611973},
           {4, -2.861475143549778}, {5, -2.8616564589740334}}};
```

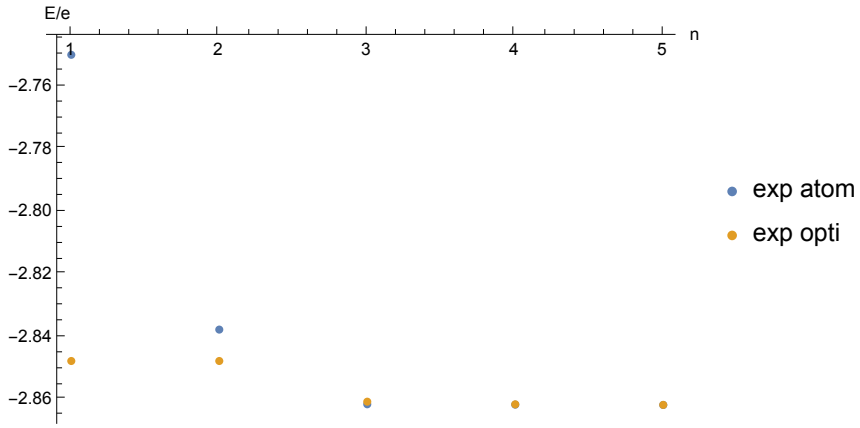
```
In[•]:= TableForm[Table[{n, temp⟦1, n, 2⟧, temp⟦2, n, 2⟧}, {n, Length[temp⟦1⟧]}],
         TableHeadings → {None, {"n", "exp atom", "exp opt"}}]
```

Out[•]//TableForm=

n	exp atom	exp opt
1	-2.75	-2.84766
2	-2.83764	-2.84766
3	-2.86146	-2.86063
4	-2.86158	-2.86148
5	-2.86168	-2.86166

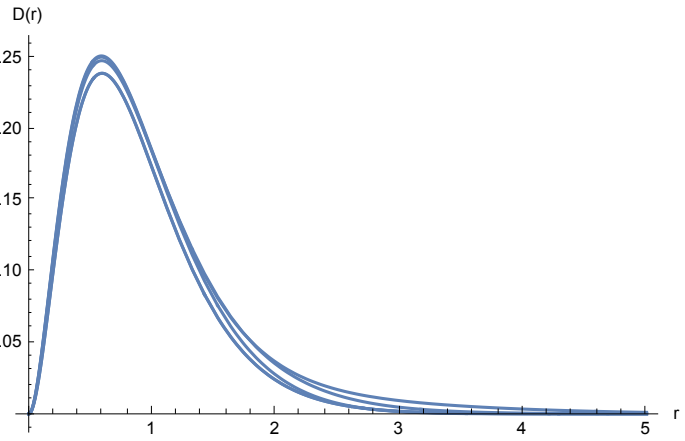
```
In[•]:= ListPlot[temp, AxesLabel → {"n", "E/e"},
         PlotLegends → {"exp atom", "exp opti"}, PlotRange → All]
```

Out[•]=



In[•]:=
```
Show[tempp7]
```

Out[•]=



La dependencia lineal de las funciones auxiliares.

3.C.5. La interacción de configuraciones para el estado singulete del helio.

Dos funciones de configuración del tipo singulete con orbitales hidrogenoides..
Psi = a * (Phi_0 + c * Phi_1)
Phi_0 = D_1
Phi_1 = (D_2 - D_3) / Sqrt[2]

La matriz del hamiltoniano.

La norma y la energía.

Las soluciones

In[•]:=
```
solci = Solve[D[eci, cci] == 0, cci];
```

In[•]:=
```
solci /. Z → 2 // N
```

Out[•]=
```
{{cci → -0.31827}, {cci → 3.14198}}
```

In[•]:=
```
(eci /. Z → 2) /. N[solci /. Z → 2]
```

Out[•]=
```
{-2.83044, -1.95591}
```

Las componentes de la energía.

El escalamiento virial.

CI + escala

In[•]:=
```
(-vci^2 / tci * 0.25 /. Z → 2) /. N[solci /. Z → 2]
```

Out[•]=
```
{-2.83989, -2.09652}
```

CI

In[•]:=
```
(Simplify[tci + vci] /. Z → 2) /. N[solci /. Z → 2]
```

Out[•]=
```
{-2.83044, -1.95591}
```

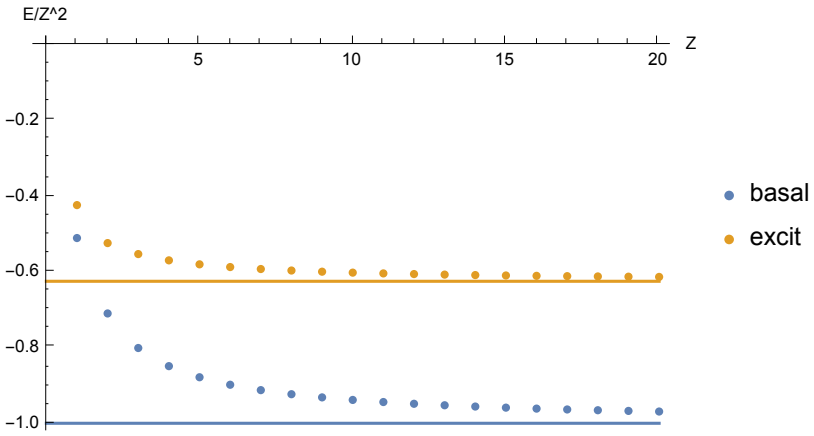
HF

```
In[•]:= {eci1, ehid[1, Z] + ehid[2, z] + Js[n1s, n2s], eci2} /. Z → 2 // N
Out[•]= {-2.75, -2.08025, -2.03635}
```

La dependencia con el número atómico.

```
In[•]:= eciz = (-vci^2 / tci * 0.25 ) /. N[solci];

In[•]:= Show[ListPlot[{Table[{z, N[eciz[[1]] /. Z → z] / z^2}, {z, 20}],
    Table[{z, N[eciz[[2]] /. Z → z] / z^2}, {z, 20}]},
  PlotLegends → {"basal", "excit"}, AxesLabel → {"Z", "E/Z^2"}],
 Plot[{-1, -5 / 8}, {z, 0, 20}]]
```

Out[•]=



4. La estructura molecular.

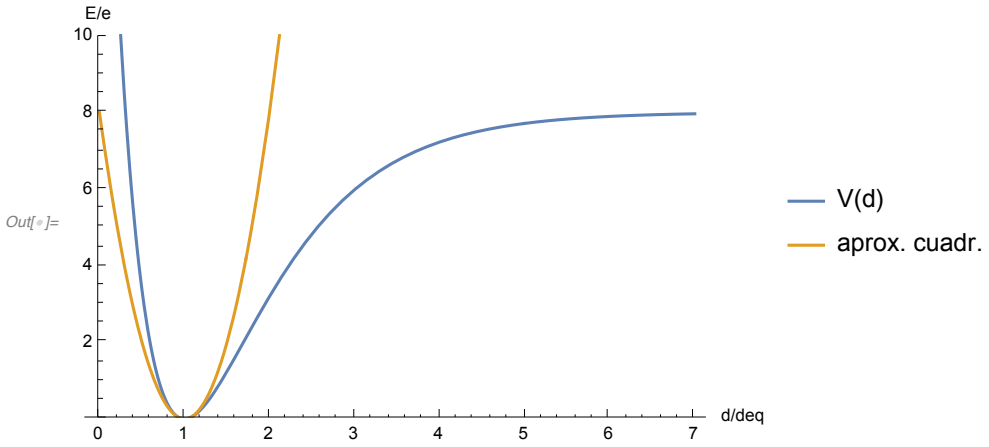
4.A. La aproximación de Born y Oppenheimer.

4.A.1. La superficie de energía potencial de una molécula diatómica.

La aproximación armónica.

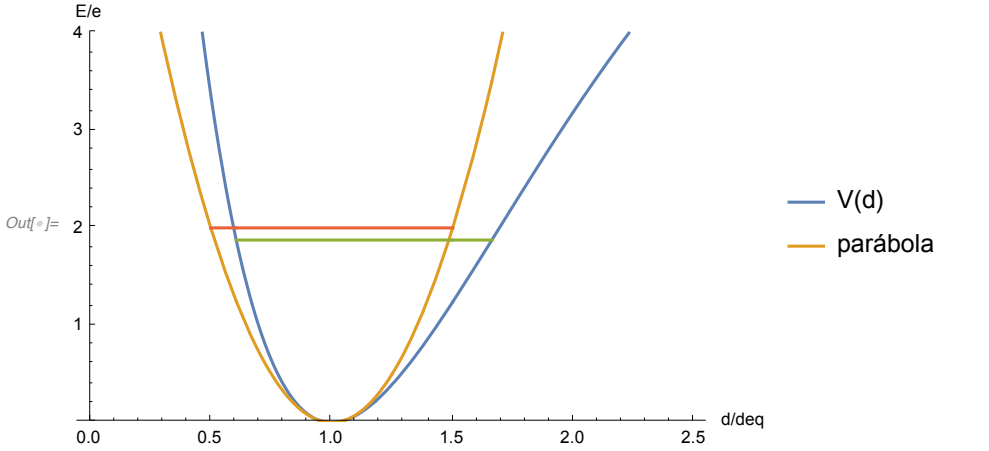
In[•]:=
```
Plot[{8 * (1 - Exp[1 - x]) ^ 2, 8 * (x - 1) * (x - 1)}, {x, 0, 7}, PlotRange → {0, 10},
 AxesLabel → {"d/deq", "E/e"}, PlotLegends → {"V(d)", "aprox. cuadr."}]
```

Out[•]=



In[•]:=
```
Plot[{8 * (1 - Exp[1 - x]) ^ 2, 8 * (x - 1) * (x - 1),
  If[x > 1 - Log[1 + Sqrt[15] / 8] && x < 1 - Log[1 - Sqrt[15] / 8], 15 / 8],
  If[x > 1 / 2 && x < 3 / 2, 2]}, {x, 0, 2.5}, PlotRange → {0, 4},
 AxesLabel → {"d/deq", "E/e"}, PlotLegends → {"V(d)", "parábola"}]
```

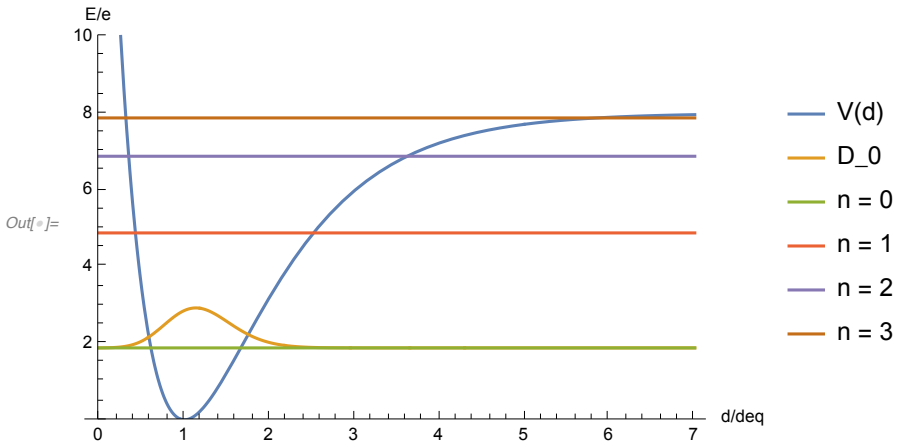
Out[•]=



Los estados cuánticos de la superficie de potencial.

In[•]:=
```
Plot[{8 * (1 - Exp[1 - x]) ^ 2,
  0.4 * 2 ^ 16 / 9 * Exp[-7 * (x - 1) - 8 * Exp[1 - x]] + 15 / 8, 15 / 8, 39 / 8, 55 / 8, 63 / 8},
 {x, 0, 7}, PlotRange → {0, 10}, AxesLabel → {"d/deq", "E/e"},
 PlotLegends → {"V(d)", "D_0", "n = 0", "n = 1", "n = 2", "n = 3"}]
```

Out[•]=



4.B. El método de Hartree y Fock molecular.

4.B.1. El ion molecular H2+.

Las funciones.

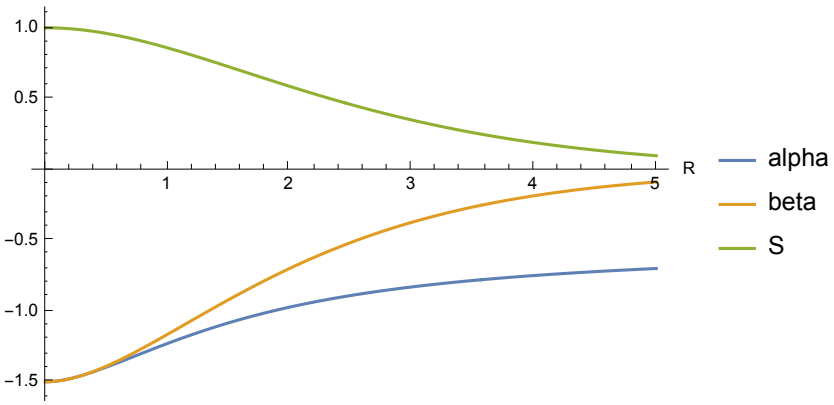
Las componentes de la energía.

In[•]:=
```
min2h2p = FindRoot[D[gh2p[R, 1, 1], R] - 1 / R^2 == 0, {R, 2}];
Print["Minimun at: ", min2h2p]
Print["E[R_min,z]= ", gh2p[R, 1, 1] /. min2h2p]
Print["W[R_min,z]= ", (gh2p[R, 1, 1] + 1 / R) /. min2h2p]
```

```
Minimun at: {R → 2.49283}
E[R_min,z]= -0.965981
W[R_min,z]= -0.564831
```

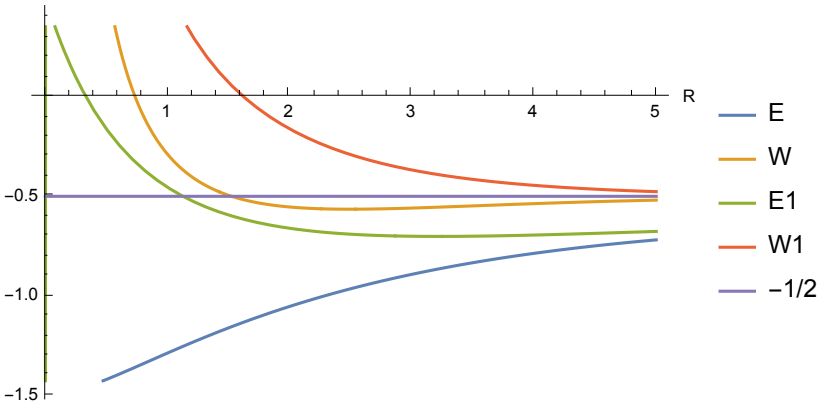
```
In[•]:= Plot[{alfah2p[R, 1, 1], betah2p[R, 1, 1], eseh2p[R, 1]},
  {R, 0, 5}, PlotLegends → {"alpha", "beta", "S"}, AxesLabel → {"R"}]
```

Out[•]=



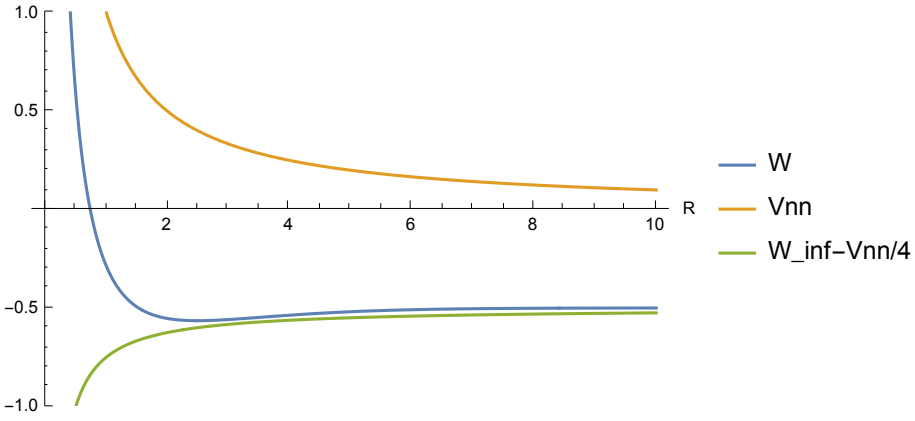

```
In[•]:= Plot[{gh2p[R, 1, 1], gh2p[R, 1, 1] + 1 / R, wh2p[R, 1, 1], wh2p[R, 1, 1] + 1 / R, -0.5},
  {R, 0, 5}, AxesLabel → {"R"}, PlotLegends → {"E", "W", "E1", "W1", "-1/2"}]
```

Out[•]=




```
In[•]:= Plot[{gh2p[R, 1, 1] + 1 / R, 1 / R, -0.5 - 0.25 / R}, {R, 0, 10}, AxesLabel → {"R"},
  PlotLegends → {"W", "Vnn", "W_inf-Vnn/4"}, PlotRange → {-1, 1}]
```

Out[•]=



4.B.2. Los orbitales moleculares de la molécula de hidrógeno.

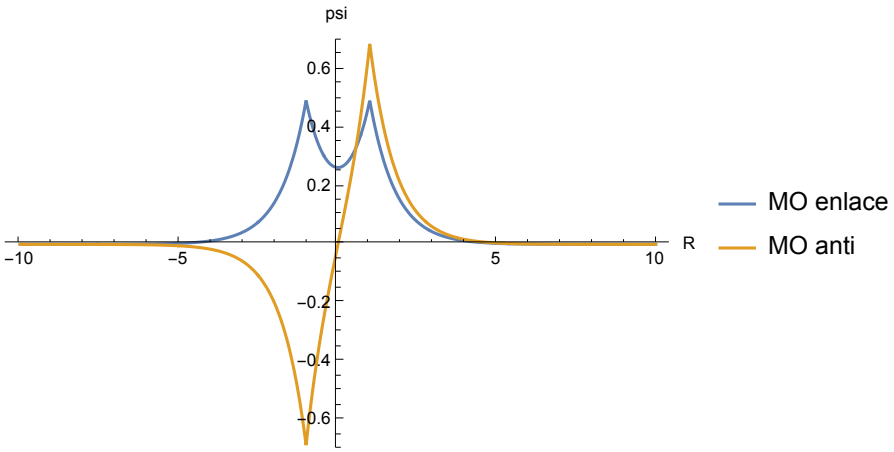
Orbitals

2 D plots

a = a_min

In[•]:=
```
Plot[{mobh2[{0, 0, r}, a /. minh21, R /. minh21],
  moah2[{0, 0, r}, a /. minh21, R /. minh21]}, {r, -10, 10}, PlotRange → {-0.7, 0.7},
 AxesLabel → {"R", "psi"}, PlotLegends → {"MO enlace", "MO anti"}]
```

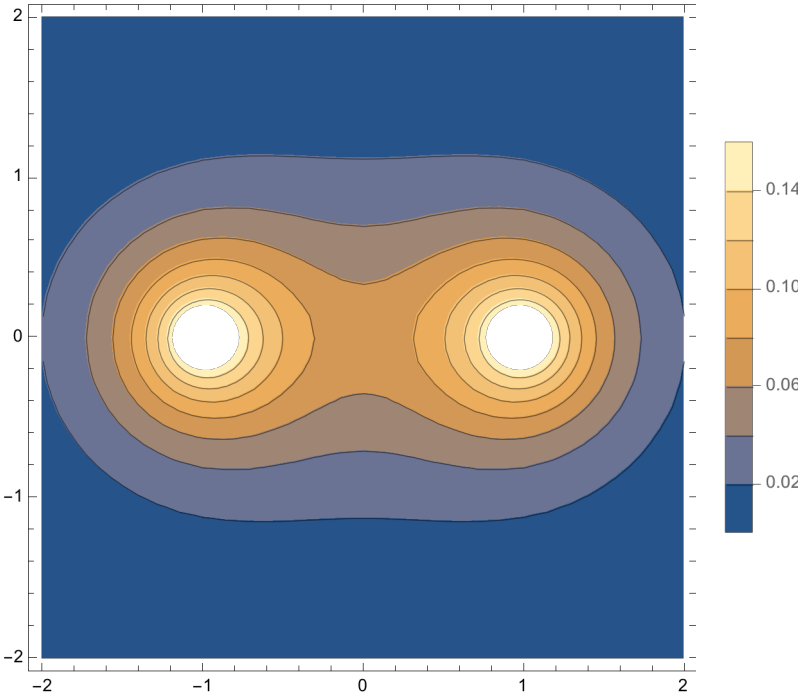
Out[•]=



El orbital de enlace.

In[•]:=
```
ContourPlot[mobh2[{0, y, r}, a /. minh21, R /. minh21]^2, {r, -2, 2},
 {y, -2, 2}, AxesLabel → {"y", "r"}, PlotLegends → Automatic]
```

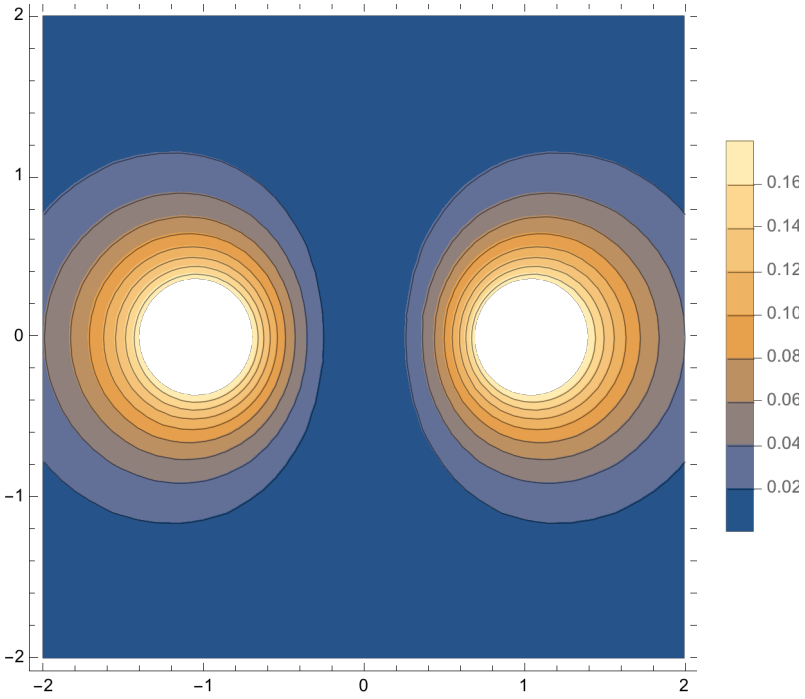
Out[•]=



El orbital de antienlace.

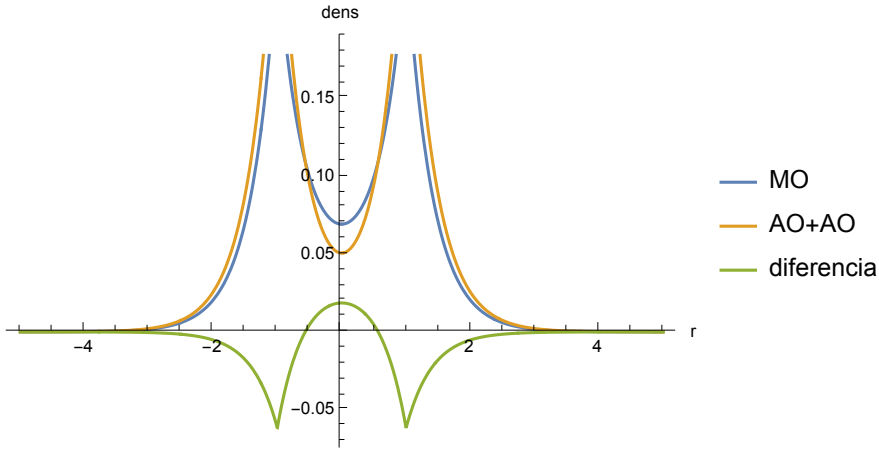
In[•]:=
```
ContourPlot[moah2[{0, y, r}, a /. minh21, R /. minh21]^2, {r, -2, 2},
 {y, -2, 2}, AxesLabel → {"y", "r"}, PlotLegends → Automatic]
```

Out[•]=



In[•]:=
```
Plot[{mobh2[{0, 0, r}, a /. minh21, R /. minh21]^2,
   (aoh[{0, 0, r} - RA[R /. minh21], a /. minh21]^2 +
      aoh[{0, 0, r} + RA[R /. minh21], a /. minh21]^2) / 2,
  mobh2[{0, 0, r}, a /. minh21, R /. minh21]^2 -
   (aoh[{0, 0, r} - RA[R /. minh21], a /. minh21]^2 +
      aoh[{0, 0, r} + RA[R /. minh21], a /. minh21]^2) / 2}, {r, -5, 5},
 AxesLabel → {"r", "dens"}, PlotLegends → {"MO", "AO+AO", "diferencia"}]
```

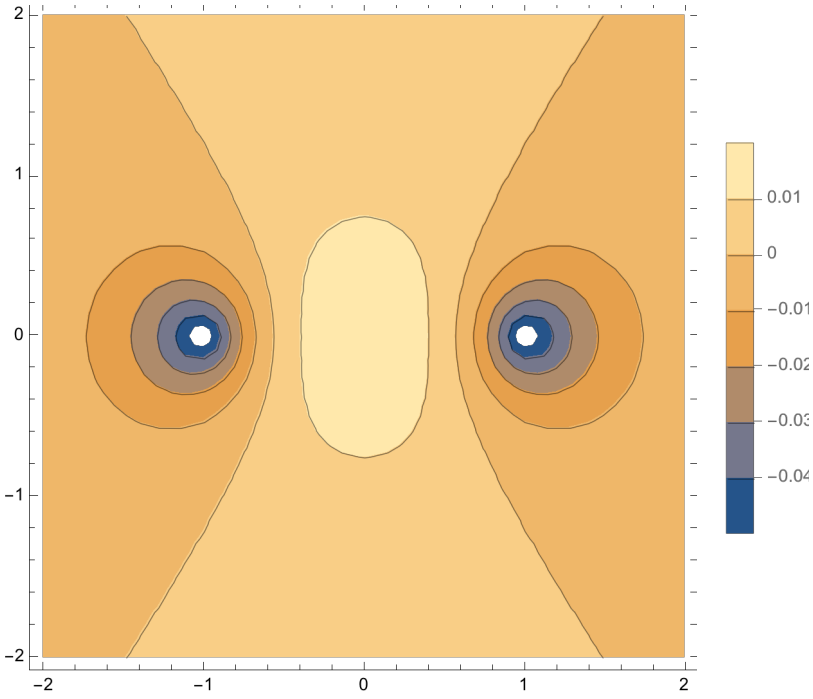
Out[•]=



La diferencia de la densidad molecular y los átomos por separado.

In[•]:=
```
ContourPlot[mobh2[{0, y, r}, a /. minh21, R /. minh21]^2 -
   (aoh[{0, y, r} - RA[R /. minh21], a /. minh21]^2 +
      aoh[{0, y, r} + RA[R /. minh21], a /. minh21]^2) / 2, {r, -2, 2},
 {y, -2, 2}, PlotRange → {-0.05, 0.05}, PlotLegends → Automatic]
```

Out[•]=



4.C. El método de Hückel.

Las constantes.

Heteroatom relative shifts (only N, O)

In[•]:=
```
kHn = 0.5;
kHo = 0.8;
kHx = 3 / Sqrt[2];
```

La conectividad de algunas moléculas.

El 1,3-butadieno

In[•]:=
```
nHpi = 4;
bondspi = {{1, 2}, {2, 3}, {3, 4}};
lHn = {};
lHo = {};
lHx = {};
```

1,3,5-Hexatriene

Six-member cycle: benzene

Pyridine

Nitrobenzene

Pyrrole

Two six-member fused cycles: naphtalene

quinoline

Three six-member fused cycles: antracene

Four six-member fused cycles

H2C=CH-X:

La construcción de la matriz de Hückel.

La matriz de Hückel.

```
In[•]:= MatrixForm[MHpi]
```

Out[•]//MatrixForm=

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

La solución de la ecuación de valores propios.

```
In[•]:= solHpi = Eigensystem[MHpi];
        cHpi = Orthogonalize[N[solHpi[[2]]]];
        indHpi = SortBy[Range[nHpi], -N[solHpi[[1]][[#]] &]
Out[•]= {2, 4, 3, 1}
```

La ocupación de los orbitales moleculares.

Los orbitales se ocupan en orden decreciente del valor propio (E = a - |b| x).
(Esto se debe hacer a mano! Los valores iguales a cero no son necesarios.)
Los valores propios de la matriz de Hückel son:

```
In[•]:= Table[solHpi[[1]][[indHpi[[i]]], {i, nHpi}] // N
Out[•]= {1.61803, 0.618034, -0.618034, -1.61803}

In[•]:= occHpi = {2, 2, 0, 0};
```

Algunas propiedades electrónicas.

La matriz de la densidad.

In[•]:=
```
locHpi = Length[occHpi];
If[locHpi < nHpi, occHpi = Join[occHpi, Table[0, {i, nHpi - locHpi}]]];
neHpi = Sum[occHpi[[i]], {i, nHpi}];
Print["Número de electrones: ", neHpi]
densHpi =
  Table[Sum[occHpi[[k]] * cHpi[[indHpi[[k]]]][[i]] * cHpi[[indHpi[[k]]]][[j]], {k, nHpi}],
   {i, nHpi}, {j, nHpi}];
Print["La matriz de la densidad: ", MatrixForm[densHpi] // N]
Print["La población en cada átomo: ", Table[densHpi[[i, i]], {i, nHpi}] // N]
```

```
Número de electrones: 4
```

La matriz de la densidad:
$$\begin{pmatrix} 1. & 0.894427 & 0. & -0.447214 \\ 0.894427 & 1. & 0.447214 & 0. \\ 0. & 0.447214 & 1. & 0.894427 \\ -0.447214 & 0. & 0.894427 & 1. \end{pmatrix}$$

```
La población en cada átomo: {1., 1., 1., 1.}
```

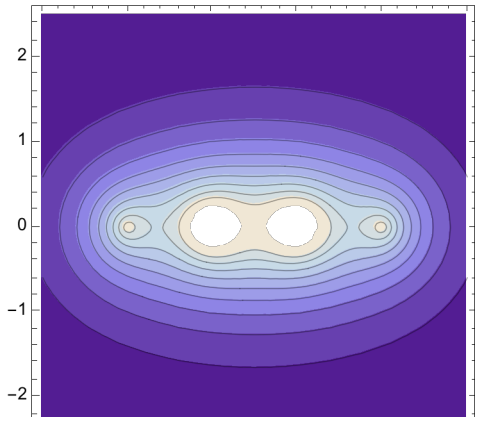
In[•]:=
```
Print["Energía_pi= ", N[Sum[occHpi[[i]] * solHpi[[1]][[indHpi[[i]]], {i, nHpi}]]]
Print["Los coeficientes de los orbitales moleculares (en renglones): ",
 MatrixForm[Table[cHpi[[indHpi[[i]]], {i, nHpi}]]]
```

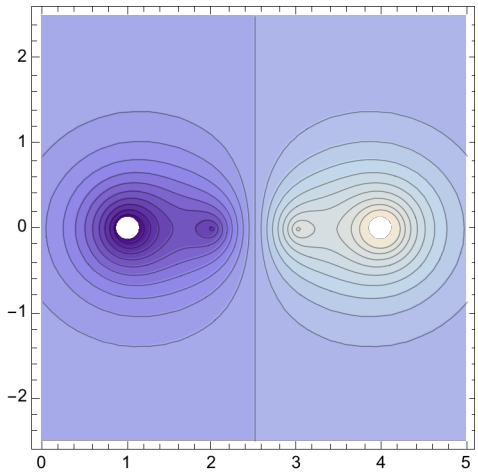
```
Energía_pi= 4.47214

Los coeficientes de los orbitales moleculares (en renglones):
```

$$\begin{pmatrix} 0.371748 & 0.601501 & 0.601501 & 0.371748 \\ -0.601501 & -0.371748 & 0.371748 & 0.601501 \\ 0.601501 & -0.371748 & -0.371748 & 0.601501 \\ -0.371748 & 0.601501 & -0.601501 & 0.371748 \end{pmatrix}$$

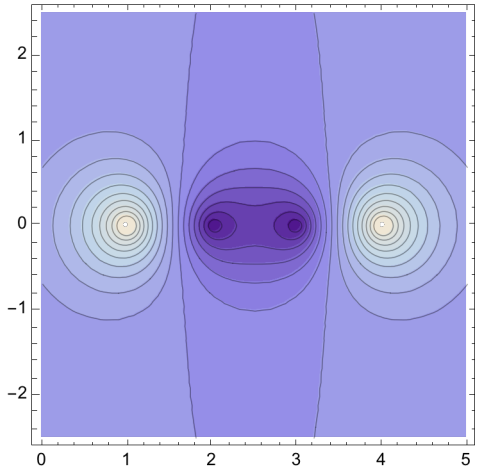
Los orbitales moleculares.

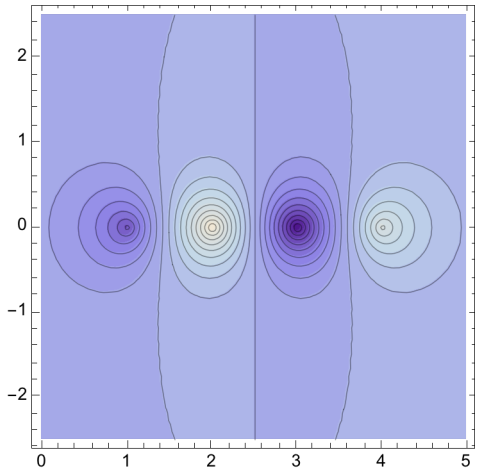
In[•]:=
```
GraphicsGrid[Table[{ContourPlot[cHpi[[indHpi[[i]]]].Table[Exp[-2 *
          Sqrt[(x - j) * (x - j) + y * y]], {j, nHpi}],
     {x, 0, nHpi + 1}, {y, -(nHpi + 1) / 2, (nHpi + 1) / 2}, Contours → 20,
     PlotRange → {-0.5, 0.5}, PlotTheme → "Classic"]}, {i, nHpi}]]
```





Out[ ]=





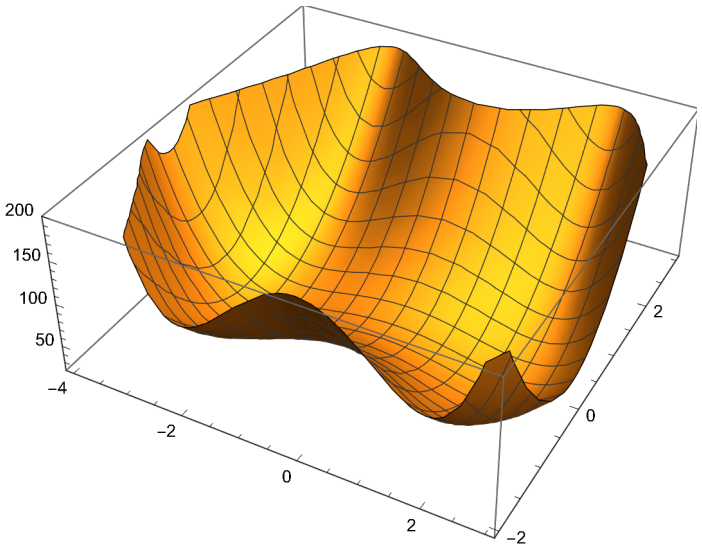
4.D. La superficie de energía potencial de las moléculas poliatómicas.

4.D.1. Un modelo de la superficie de energía potencial.

In[•]:=
```
pespoly[x_, y_] := (y * y + 1) * (x * x * x * x - 8 * x * x + 40);
```

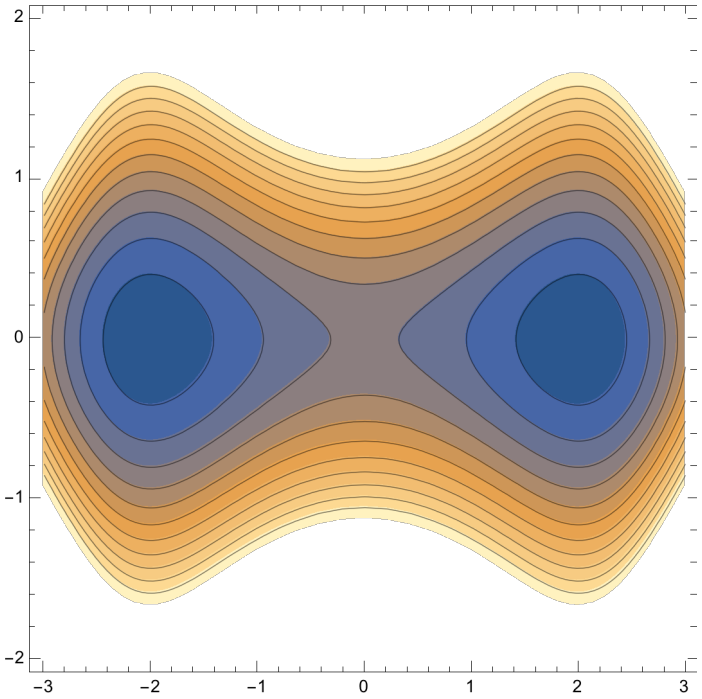
In[•]:=
```
Plot3D[pespoly[x, y], {x, -4, 3}, {y, -2, 3},
 PlotRange → {20, 200}, ClippingStyle → None]
```

Out[•]=



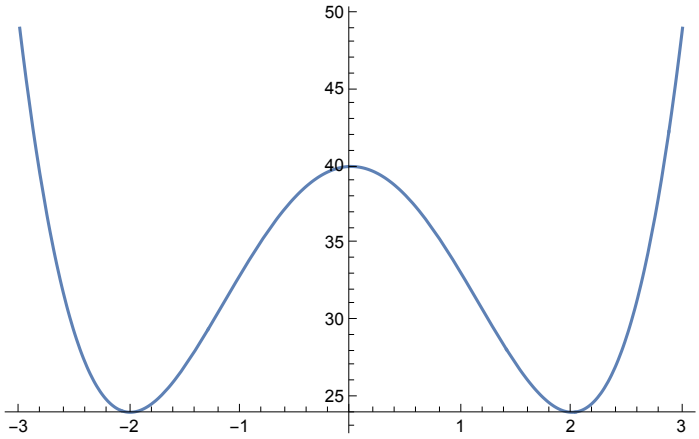
In[•]:=
```
ContourPlot[pespoly[x, y], {x, -3, 3},
 {y, -2, 2}, PlotRange → {0, 90}, Contours → 15]
```

Out[•]=



In[•]:=
```
Plot[pespoly[x, 0], {x, -3, 3}]
```

Out[•]=



El estado de transición.

In[•]:=
```
Print["TS: ", tsleps =
  FindRoot[{D[pespoly[x, y], x] == 0, D[pespoly[x, y], y] == 0}, {x, 0}, {y, 1}]]
Print["Energía en el TS: ", pespoly[x, y] /. tsleps]
Print["grad_PES: ", {D[pespoly[x, y], x], D[pespoly[x, y], y]} /. tsleps]
Print["Valores propios de la matriz Hessiana en el TS: ",
 Eigenvalues[{{D[pespoly[x, y], {x, 2}], D[pespoly[x, y], {x, 1}, {y, 1}]},
    {D[pespoly[x, y], {x, 1}, {y, 1}], D[pespoly[x, y], {y, 2}]}} /. tsleps]]
```

```
TS: {x → 0., y → 0.}
Energía en el TS: 40.
grad_PES: {0., 0.}
Valores propios de la matriz Hessiana en el TS: {80., -16.}
```

Los mínimos en la superficie de potencial.

In[•]:=
```
Print["Mínimo 1: ", tsleps =
  FindRoot[{D[pespoly[x, y], x] == 0, D[pespoly[x, y], y] == 0}, {x, 3}, {y, 1}]]
Print["Energía en el mínimo: ", pespoly[x, y] /. tsleps]
Print["grad_PES: ", {D[pespoly[x, y], x], D[pespoly[x, y], y]} /. tsleps]
Print["Valores propios de la matriz Hessiana en el mínimo: ",
 Eigenvalues[{{D[pespoly[x, y], {x, 2}], D[pespoly[x, y], {x, 1}, {y, 1}]},
    {D[pespoly[x, y], {x, 1}, {y, 1}], D[pespoly[x, y], {y, 2}]}} /. tsleps]]
```

```
Mínimo 1: {x → 2., y → 0.}
Energía en el mínimo: 24.
grad_PES: {0., 0.}
Valores propios de la matriz Hessiana en el mínimo: {48., 32.}
```

In[•]:=
```
Print["Mínimo 2: ", tsleps =
  FindRoot[{D[pespoly[x, y], x] == 0, D[pespoly[x, y], y] == 0}, {x, -3}, {y, 1}]]
Print["Energía en el mínimo: ", pespoly[x, y] /. tsleps]
Print["grad_PES: ", {D[pespoly[x, y], x], D[pespoly[x, y], y]} /. tsleps]
Print["Valores propios de la matriz Hessiana en el mínimo: ",
 Eigenvalues[{{D[pespoly[x, y], {x, 2}], D[pespoly[x, y], {x, 1}, {y, 1}]},
    {D[pespoly[x, y], {x, 1}, {y, 1}], D[pespoly[x, y], {y, 2}]}} /. tsleps]]
```

```
Mínimo 2: {x → -2., y → 0.}
Energía en el mínimo: 24.
grad_PES: {0., 0.}
Valores propios de la matriz Hessiana en el mínimo: {48., 32.}
```

4.D.2. El modelo LEPS.

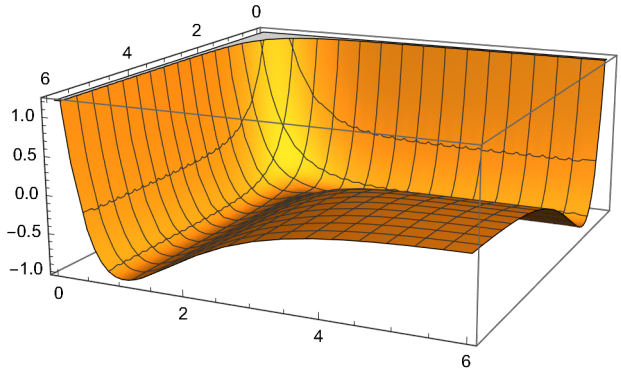
Las funciones.

La superficie de energía potencial de una reaccción simétrica

In[•]:=
```
parleps = {{1, 1, 1}, {1, 1, 1}, {1, 1, 1}};
```

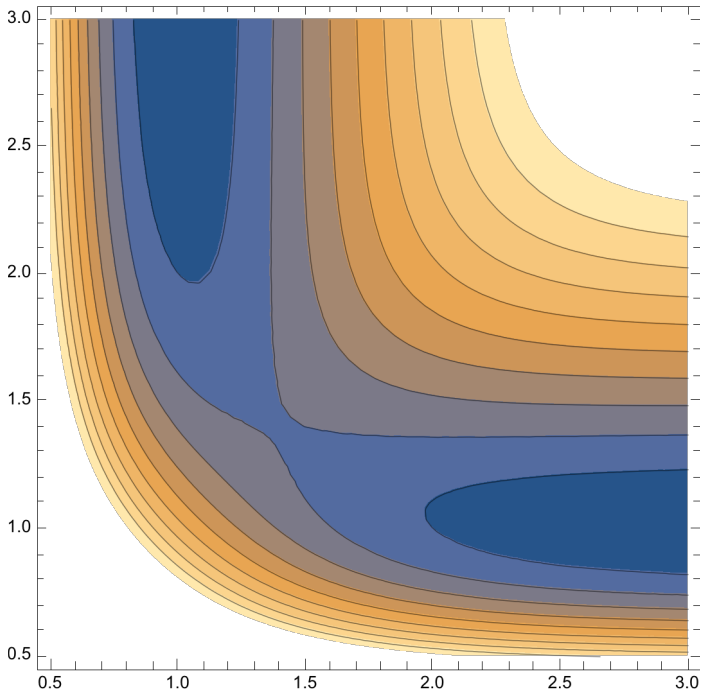
In[•]:=
```
Plot3D[leps[r, s, parleps, 0.18], {s, 0, 6}, {r, 0, 6}]
```

Out[•]=



In[•]:=
```
ContourPlot[leps[r, s, parleps, 0.18],
 {s, 0.5, 3}, {r, 0.5, 3}, PlotRange → {-1.0, -0.5}]
```

Out[•]=



- El estado de transición.

In[•]:=
```
Print["TS: ", tsleps = FindRoot[{D[leps[r, s, parleps, 0.18], r] == 0,
    D[leps[r, s, parleps, 0.18], s] == 0}, {r, 1.3}, {s, 1.3}]]
Print["Energía en el TS: ", leps[r, s, parleps, 0.18] /. tsleps]
Print["grad_PES: ",
 {D[leps[r, s, parleps, 0.18], r], D[leps[r, s, parleps, 0.18], s]} /. tsleps]
Print["Valores propios de la matriz Hessiana en el TS: ",
 Eigenvalues[{{D[leps[r, s, parleps, 0.18], {r, 2}],
     D[leps[r, s, parleps, 0.18], {r, 1}, {s, 1}]}, {D[leps[r, s, parleps, 0.18],
      {r, 1}, {s, 1}], D[leps[r, s, parleps, 0.18], {s, 2}]}} /. tsleps]]
```

```
TS: {r → 1.39663, s → 1.39663}
Energía en el TS: -0.901645
grad_PES: {0., 0.}
Valores propios de la matriz Hessiana en el TS: {0.930513, -0.408414}
```

- Los mínimos en la superficie de potencial.

In[•]:=
```
Print["Mínimo 1: ", tsleps = FindRoot[{D[leps[r, s, parleps, 0.18], r] == 0,
    D[leps[r, s, parleps, 0.18], s] == 0}, {r, 1}, {s, 3}]]
Print["Energía en el mínimo 1: ", leps[r, s, parleps, 0.18] /. tsleps]
Print["grad_PES: ",
 {D[leps[r, s, parleps, 0.18], r], D[leps[r, s, parleps, 0.18], s]} /. tsleps]
Print["Valores propios de la matriz Hessiana en el mínimo 1: ",
 Eigenvalues[{{D[leps[r, s, parleps, 0.18], {r, 2}],
     D[leps[r, s, parleps, 0.18], {r, 1}, {s, 1}]}, {D[leps[r, s, parleps, 0.18],
      {r, 1}, {s, 1}], D[leps[r, s, parleps, 0.18], {s, 2}]}} /. tsleps]]
```

Mínimo 1: {r → 1., s → 33.3963}

Energía en el mínimo 1: -1.

grad_PES: $\{-1.88173 \times 10^{-16}, -2.46919 \times 10^{-16}\}$

Valores propios de la matriz Hessiana en el mínimo 1: $\{2., 2.46919 \times 10^{-16}\}$

In[•]:=
```
Print["Mínimo 2: ", tsleps = FindRoot[{D[leps[r, s, parleps, 0.18], r] == 0,
    D[leps[r, s, parleps, 0.18], s] == 0}, {r, 3}, {s, 1}]]
Print["Energía en el mínimo 2: ", leps[r, s, parleps, 0.18] /. tsleps]
Print["grad_PES: ",
 {D[leps[r, s, parleps, 0.18], r], D[leps[r, s, parleps, 0.18], s]} /. tsleps]
Print["Valores propios de la matriz Hessiana en el mínimo 2: ",
 Eigenvalues[{{D[leps[r, s, parleps, 0.18], {r, 2}],
     D[leps[r, s, parleps, 0.18], {r, 1}, {s, 1}]}, {D[leps[r, s, parleps, 0.18],
      {r, 1}, {s, 1}], D[leps[r, s, parleps, 0.18], {s, 2}]}} /. tsleps]]
```

Mínimo 2: {r → 35.3972, s → 1.}

Energía en el mínimo 2: -1.

grad_PES: $\{-3.3389 \times 10^{-17}, -1.88173 \times 10^{-16}\}$

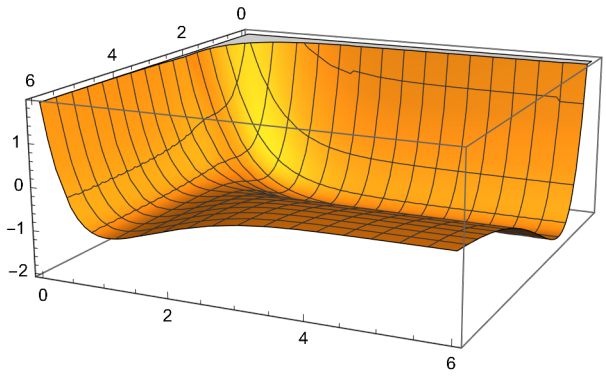
Valores propios de la matriz Hessiana en el mínimo 2: $\{2., 3.3389 \times 10^{-17}\}$

La superficie de energía potencial de una reacción asimétrica.

In[•]:=
```
parleps = {{1, 1, 1}, {2, 1.5, 0.7}, {2, 1.5, 0.7}};
```

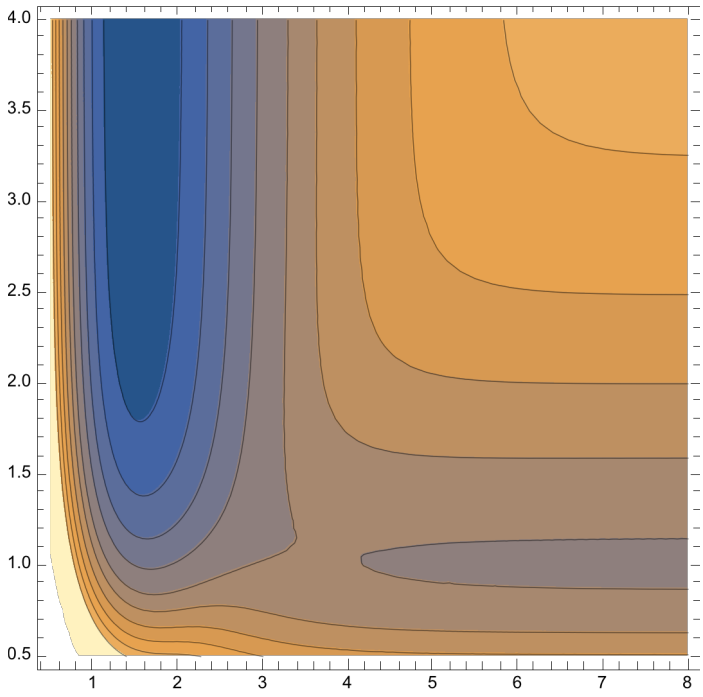
In[•]:=
```
Plot3D[leps[r, s, parleps, 0.18], {s, 0, 6}, {r, 0, 6}]
```

Out[•]=



In[•]:=
```
ContourPlot[leps[r, s, parleps, 0.18], {s, 0.5, 8}, {r, 0.5, 4},
 Contours → {0, -0.2, -0.4, -0.6, -0.8, -0.98, -1.2, -1.4, -1.6, -1.8}]
```

Out[•]=



- El estado de transición.

In[•]:=
```
Print["TS: ", tsleps = FindRoot[{D[leps[r, s, parleps, 0.18], r] == 0,
    D[leps[r, s, parleps, 0.18], s] == 0}, {r, 1}, {s, 3}]]
Print["Energía en el TS: ", leps[r, s, parleps, 0.18] /. tsleps]
Print["grad_PES: ",
 {D[leps[r, s, parleps, 0.18], r], D[leps[r, s, parleps, 0.18], s]} /. tsleps]
Print["Valores propios de la matriz Hessiana en el TS: ",
 Eigenvalues[{{D[leps[r, s, parleps, 0.18], {r, 2}],
     D[leps[r, s, parleps, 0.18], {r, 1}, {s, 1}]}, {D[leps[r, s, parleps, 0.18],
      {r, 1}, {s, 1}], D[leps[r, s, parleps, 0.18], {s, 2}]}} /. tsleps]]
```

```
TS: {r → 1.08295, s → 3.63293}
Energía en el TS: -0.974663
grad_PES: {0., 1.4113 × 10^-16}
Valores propios de la matriz Hessiana en el TS: {1.3967, -0.0907865}
```