Taller de Química Cuántica.

Material para el curso de Fisicoquímica general -estructura atómica .

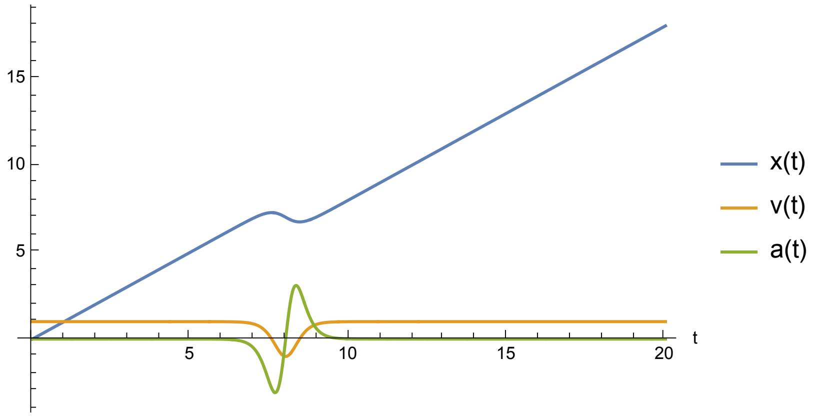
1. Los fundamentos de la mecánica cuántica.

1.A. La mecánica clásica.

1.A.1. Un ejemplo sencillo.

In[∘]:=
```
Plot[{t - Tanh[2 t - 16] - 1, 1 - D[Tanh[2 * x - 16], x] /. x → t,
  - D[Tanh[2 * x - 16], {x, 2}] /. x → t}, {t, 0, 20},
 AxesLabel → {"t"}, PlotLegends → {"x(t)", "v(t)", "a(t)"}]
```

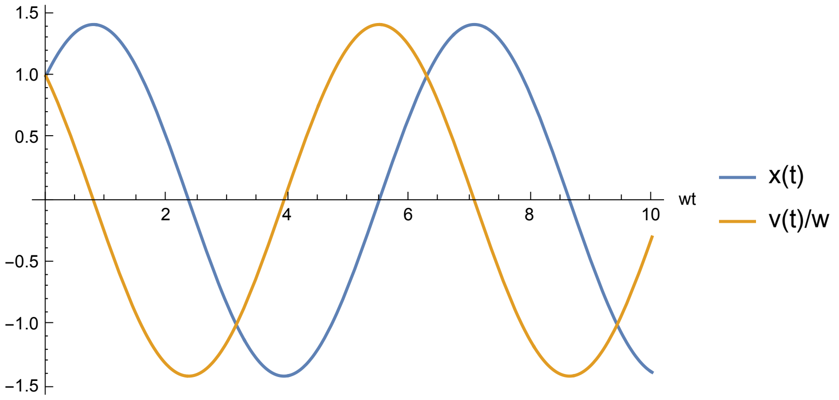
Out[∘]=



1.A.2. El oscilador armónico.

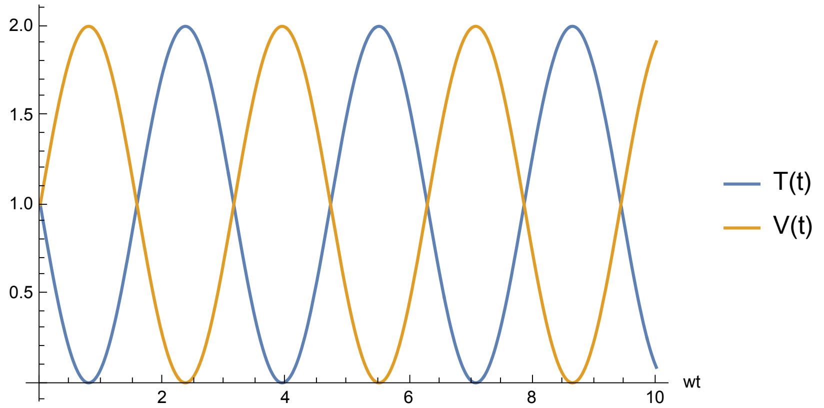
In[21]:=
```
Plot[{Cos[t] + Sin[t], -Sin[t] + Cos[t]}, {t, 0, 10},
 AxesLabel → {"wt"}, PlotLegends → {"x(t)", "v(t)/w"}]
```

Out[21]=



In[23]:=
```
Plot[{(Cos[t] - Sin[t])^2, (Sin[t] + Cos[t])^2},
 {t, 0, 10}, AxesLabel → {"wt"}, PlotLegends → {"T(t)", "V(t)"}]
```

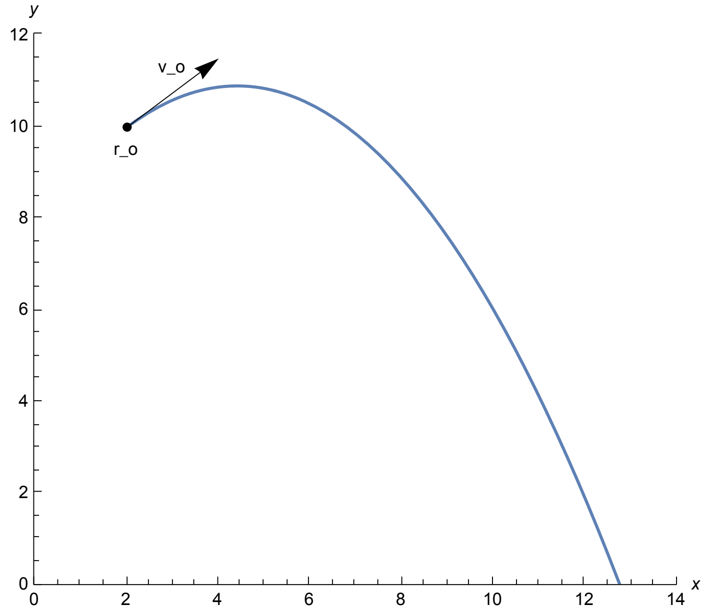
Out[23]=



1.A.3. El tiro parabólico.

In[42]:=
```
Show[ParametricPlot[{2 + 8 * t, 10 + 6 * t - 10 * t^2},
   {t, 0, 1.4}, PlotRange → {{0, 14}, {0, 12}}, AxesLabel → {x, y}],
  Graphics[{Black, Arrow[{{2, 10}, {4, 10 + 3 / 2}}]}],
  Graphics[{Black, Disk[{2, 10}, 0.1]}],
  Graphics[Text["v_o", {3, 11.3}]], Graphics[Text["r_o", {2, 9.5}]]]
```

Out[42]=

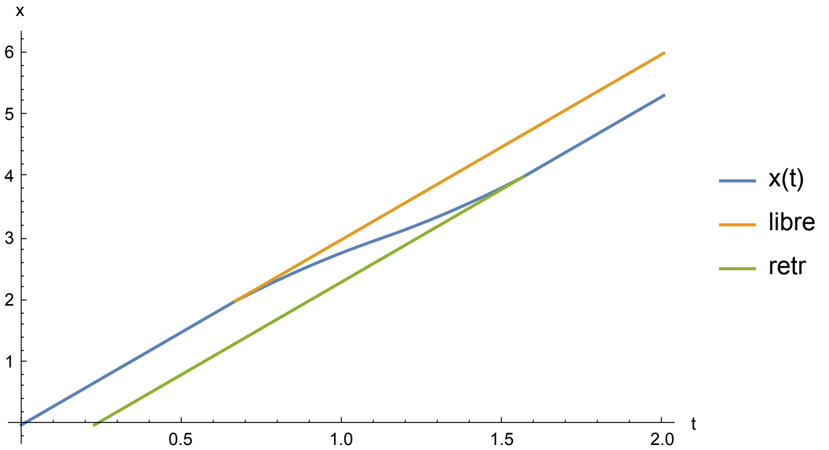


1.A.4. Una rampa doble.

La energía es suficiente para remontar la pendiente.

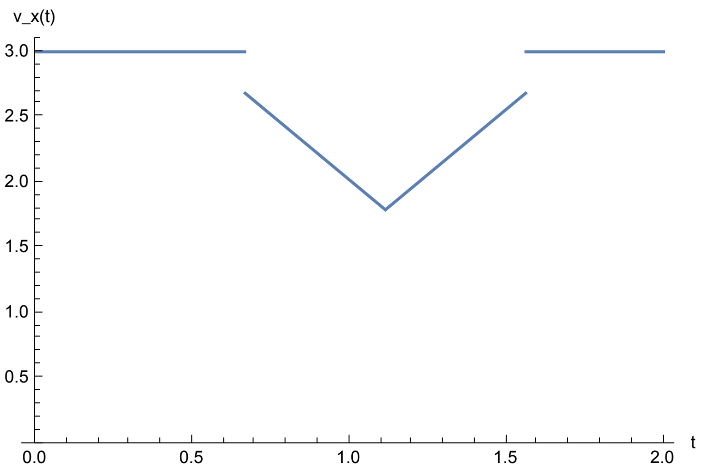
In[∘]:=
```
Plot[{
  If[t < 2 / 3, 3 * t,
   If[t < 2 / 3 + 1 / Sqrt[5], 2 + 2 / Sqrt[5] * (3 * t - 2 - Sqrt[5] / 2 * (t - 2 / 3) ^ 2),
    If[t < 2 / 3 + 2 / Sqrt[5], 3 + 2 / Sqrt[5] *
       (Sqrt[5] / 2 * (t - 2 / 3 - 1 / Sqrt[5]) ^ 2 + 2 * (t - 2 / 3 - 1 / Sqrt[5])),
     4 + 3 * (t - 2 / 3 - 2 / Sqrt[5])]]]
  , If[t > 2 / 3, 3 * t],
  If[t < 2 / 3 + 2 / Sqrt[5] && t > 2 / Sqrt[5] - 2 / 3, 4 + 3 * (t - 2 / 3 - 2 / Sqrt[5])]},
 {t, 0, 2}, PlotRange → All, AxesLabel → {"t", "x"},
 PlotLegends → {"x(t)", "libre", "retr"}]
```

Out[∘]=



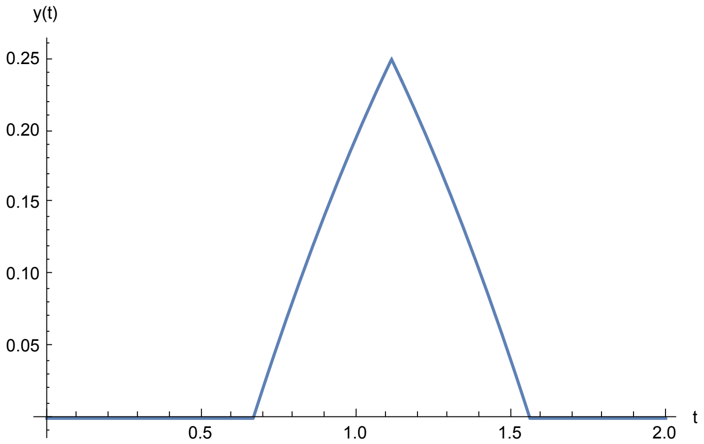
In[9]:=
```
Plot[
 If[t < 2 / 3, 3,
  If[t < 2 / 3 + 1 / Sqrt[5],
   2 / Sqrt[5] * (3 - Sqrt[5] * (t - 2 / 3)), If[t < 2 / 3 + 2 / Sqrt[5], 2 / Sqrt[5] *
     (Sqrt[5] * (t - 2 / 3 - 1 / Sqrt[5]) + 2), 3]]],
 {t, 0, 2}, PlotRange → {0, 3.1}, AxesLabel → {"t", "v_x(t)"}]
```

Out[9]=



In[∘]:=
```
Plot[{
  If[t < 2 / 3, 0,
   If[t < 2 / 3 + 1 / Sqrt[5], (2 / Sqrt[5] * (3 * t - 2 - Sqrt[5] / 2 * (t - 2 / 3) ^2)) / 4,
    If[t < 2 / 3 + 2 / Sqrt[5], (1 - 2 / Sqrt[5] *
         (Sqrt[5] / 2 * (t - 2 / 3 - 1 / Sqrt[5]) ^2 + 2 * (t - 2 / 3 - 1 / Sqrt[5]))) / 4,
     0]]]
 },
 {t, 0, 2}, PlotRange → All, AxesLabel → {"t", "y(t)"}]
```

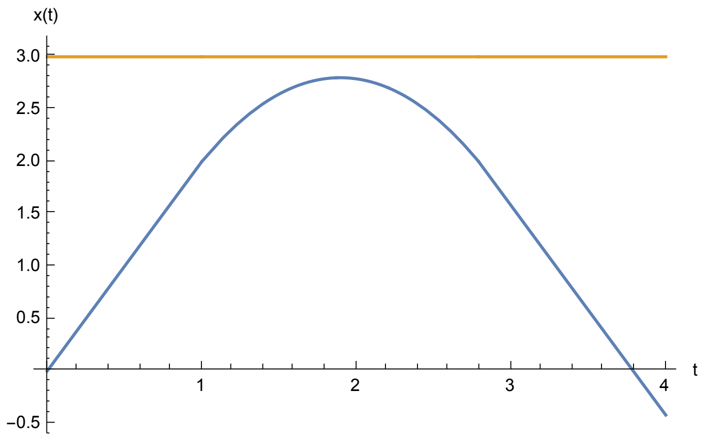
Out[∘]=



La energía es insuficiente para remontar la pendiente.

In[18]:=
```
Plot[{
  If[t < 1, 2 * t,
   If[t < 1 + 4 / Sqrt[5], 2 + ((2 * t - 2 - Sqrt[5] / 2 * (t - 1) ^2)) * 2 / Sqrt[5],
    2 - 2 * (t - 1 - 4 / Sqrt[5])]], 3},
 {t, 0, 4}, PlotRange → All, AxesLabel → {"t", "x(t)"}]
```

Out[18]=



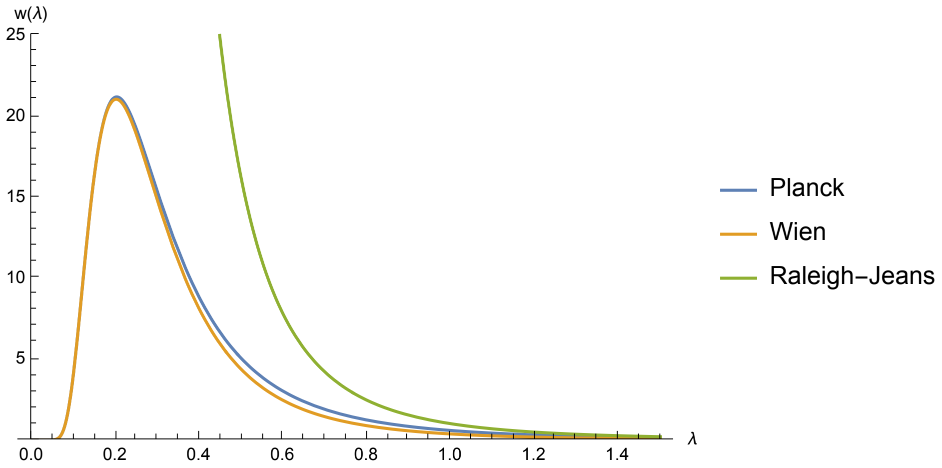
1.B.1. La radiación del cuerpo negro.

Las distribuciones.

Las gráficas.

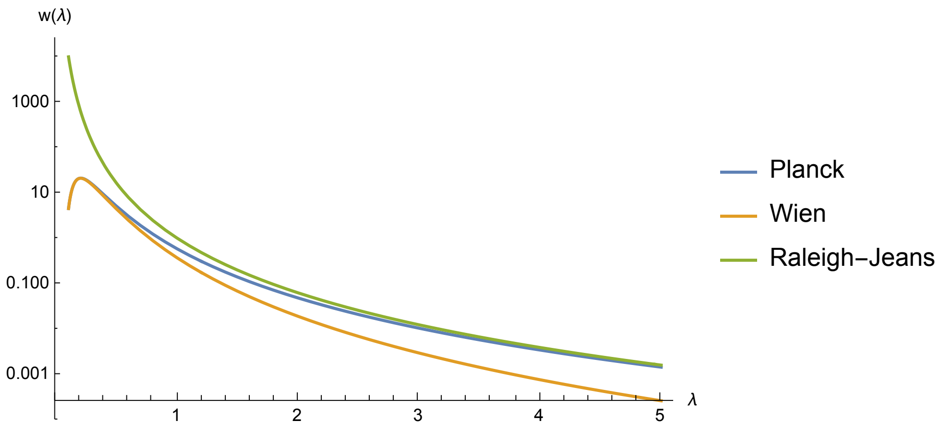
In[∘]:=
```
Plot[{wp[1, x], ww[1, x], wrj[1, x]}, {x, 0, 1.5}, PlotRange → {0, 25},
 AxesLabel → {"λ", "w(λ)"}, PlotLegends → {"Planck", "Wien", "Raleigh-Jeans"}]
```

Out[∘]=



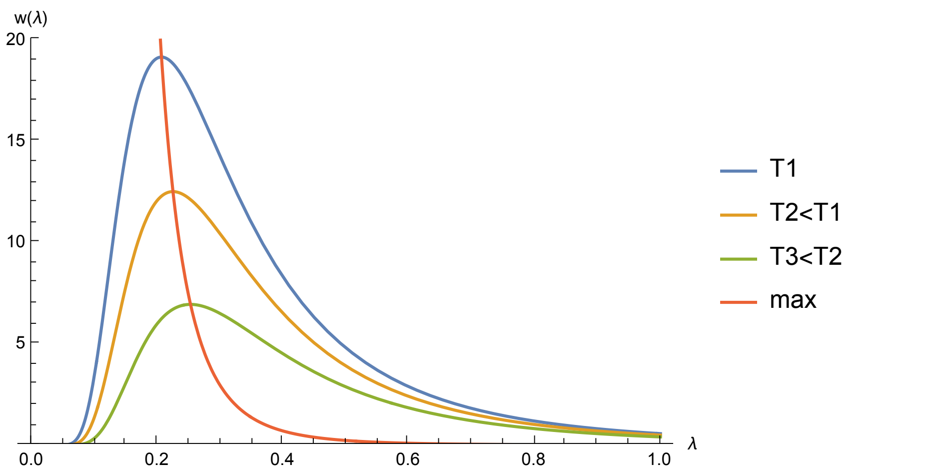
In[∘]:=
```
LogPlot[{wp[1, x], ww[1, x], wrj[1, x]}, {x, 0.1, 5},
 AxesLabel → {"λ", "w(λ)"}, PlotLegends → {"Planck", "Wien", "Raleigh-Jeans"}]
```

Out[∘]=



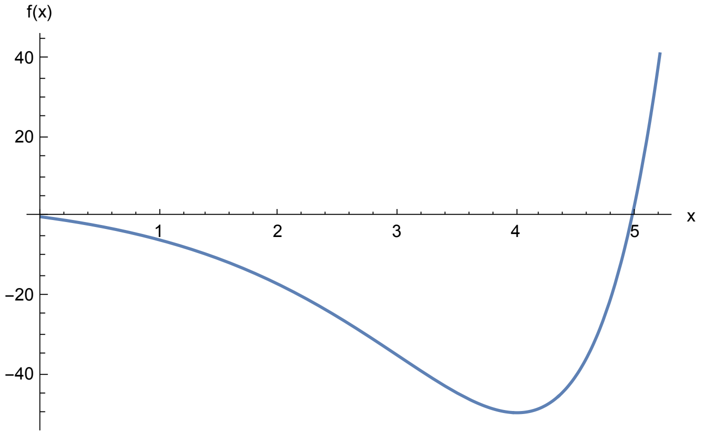
In[∘]:=
```
Plot[{wp[0.98, x], wp[0.90, x], wp[0.80, x], 1 / (x^5 * (Exp[4.965] - 1))},
 {x, 0, 1}, PlotRange → {0, 20}, AxesLabel → {"λ", "w(λ)"},
 PlotLegends → {"T1", "T2<T1", "T3<T2", "max"}]
```

Out[∘]=



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

Out[∘]=



1.C. Los principios de la teoría cuántica.

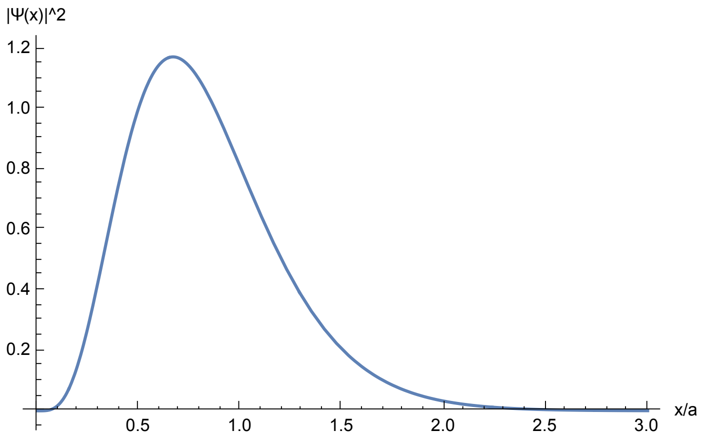
1.C.1. Las funciones de onda.

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"}]
```

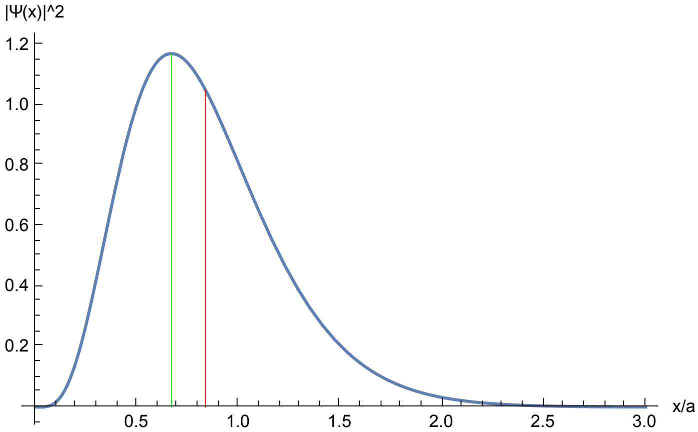
$324\, e^{-6x}\, x^4$

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}}]}]]
```

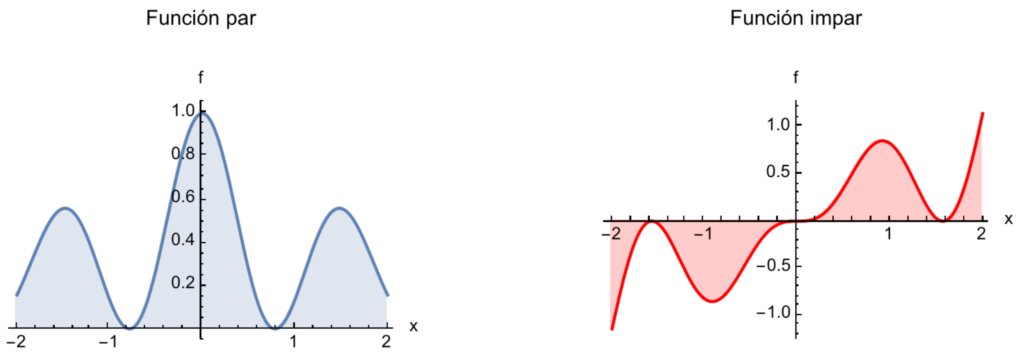
Out[∘]=



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[∘]=



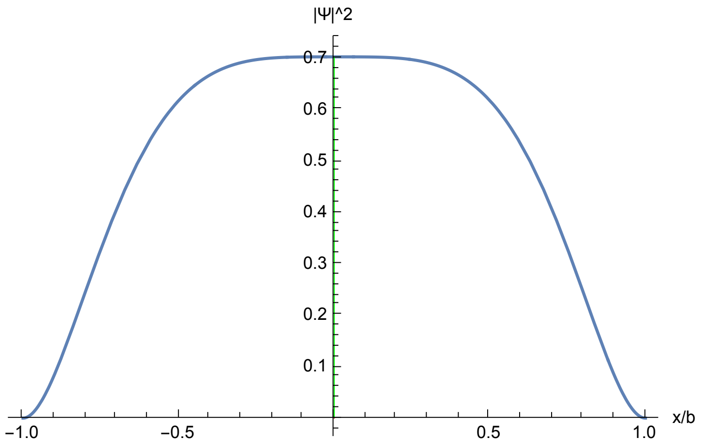
Otras densidades de probablilidad.

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}]}]]
```

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

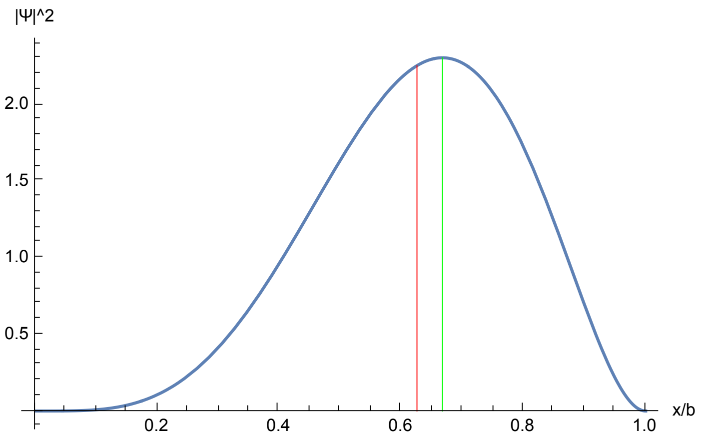
Out[∘]=



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.

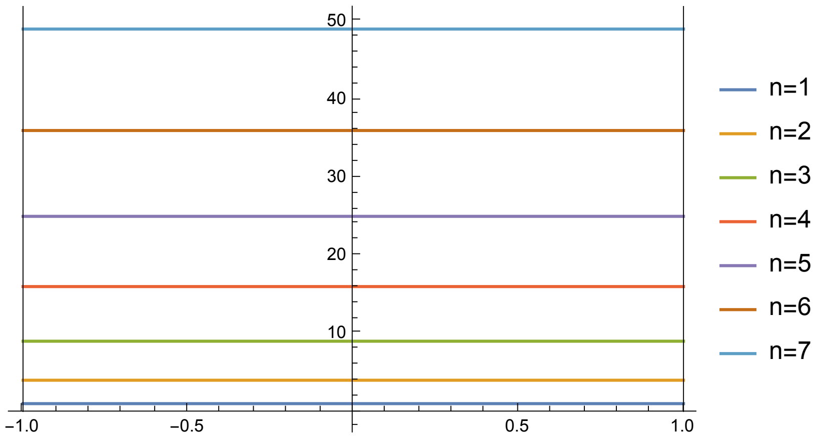
2.A. El movimiento traslacional.

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[∘]=

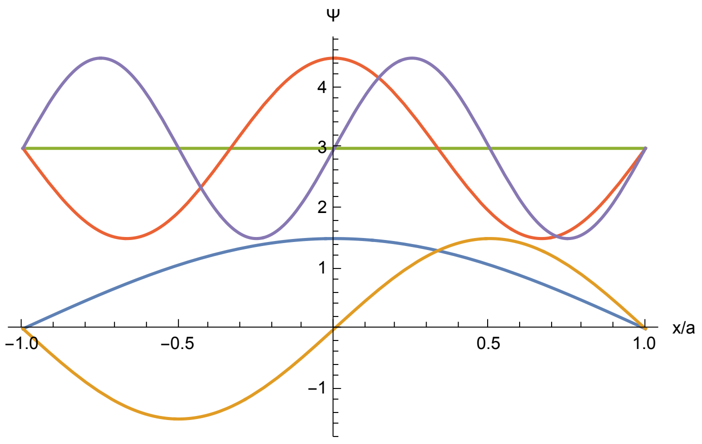


Las funciones de onda.

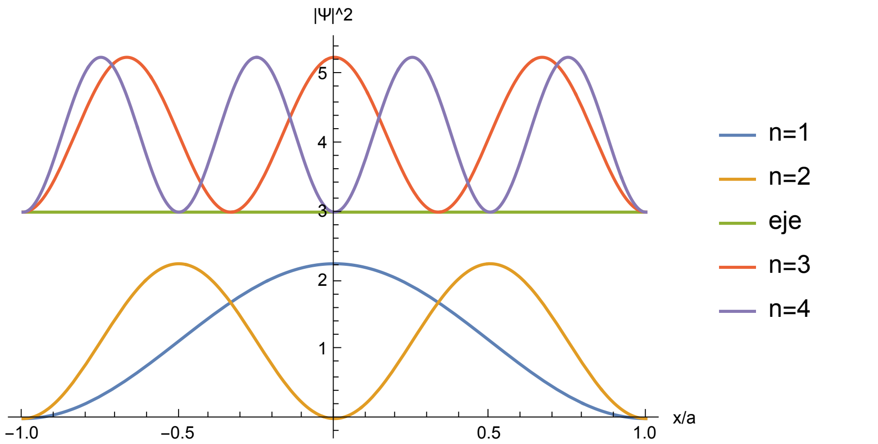
In[∘]:=
```
trfop[x_, n_, a_] := a * Cos[n * x * Pi / 2];
trfoi[x_, n_, a_] := a * Sin[n * x * Pi / 2];
```

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"}]
```

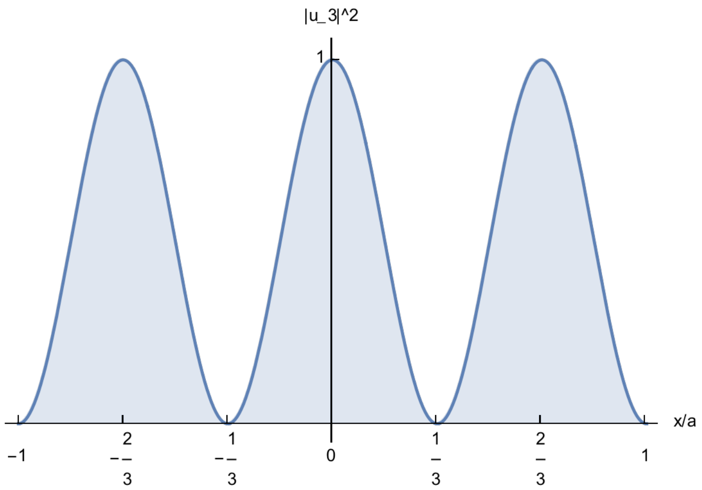
Out[∘]=



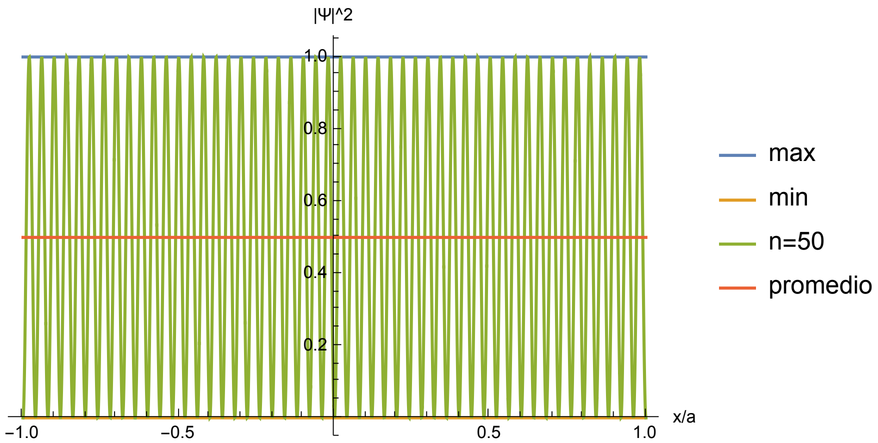
In[ ]:=
```
Plot[{trfop[x, 1, 1.5]^2, trfoi[x, 2, 1.5]^2, 3,
  trfop[x, 3, 1.5]^2 + 3, trfoi[x, 4, 1.5]^2 + 3}, {x, -1, 1},
 AxesLabel → {"x/a", "|Ψ|^2"}, PlotLegends → {"n=1", "n=2", "eje", "n=3", "n=4"}]
```

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[ ]=


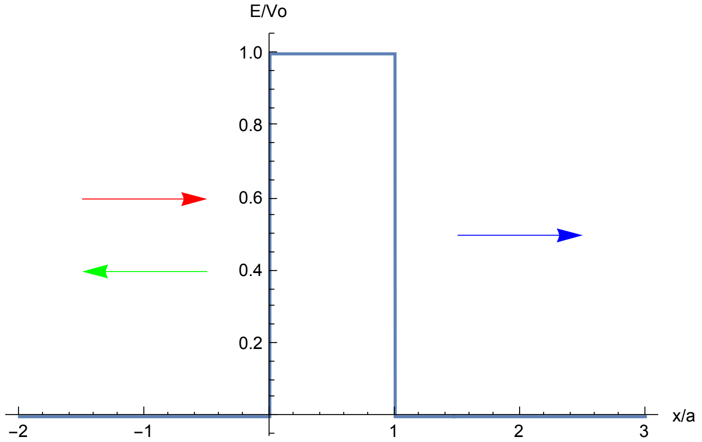
2.A.2. La barrera de potencial.

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}}]}]]
```

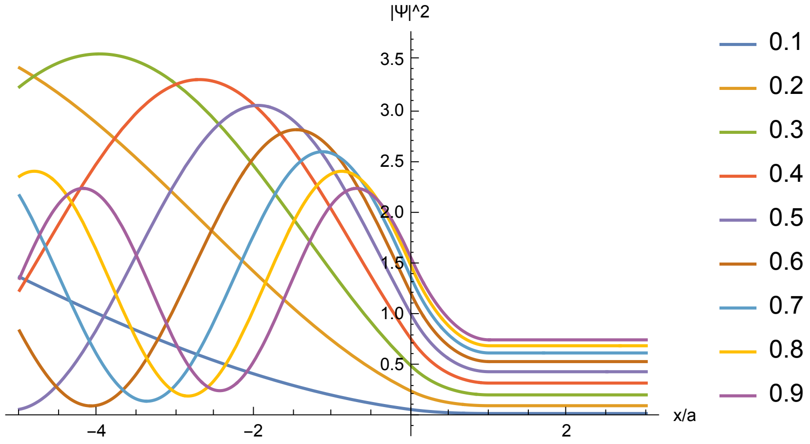
Out[∘]=



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"}]
```

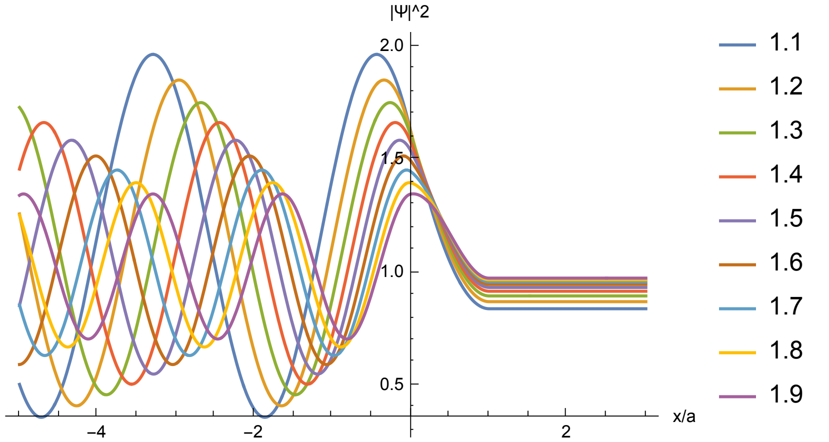
Out[∘]=



Las densidades de probabilidad para E > Vo.

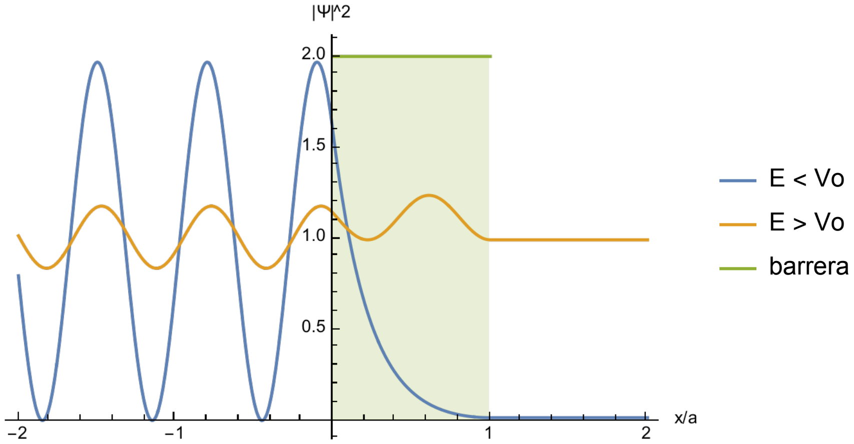
In[∘]:=
```
Plot[Evaluate[Table[P1[x, 1, 1 + 0.1 * i], {i, 9}]], {x, -5, 3},
 PlotLegends → Table[1 + 0.1 * i, {i, 9}], AxesLabel → {"x/a", "|Ψ|^2"}]
```

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}]
```

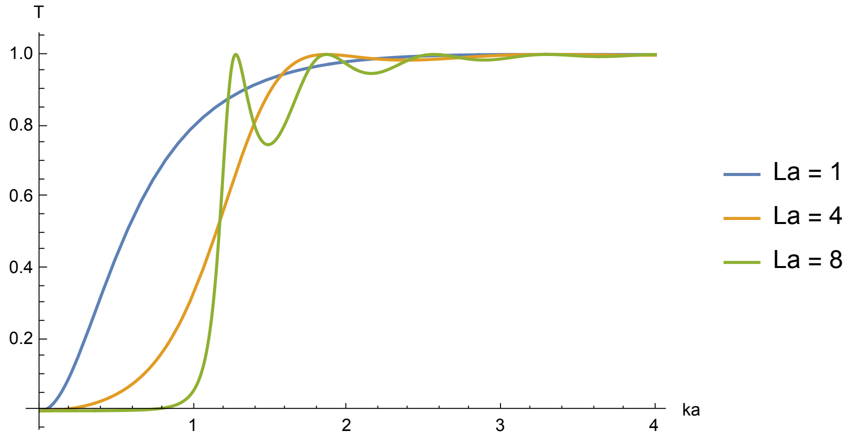
Out[∘]=



La transmisión a través de una barrera.

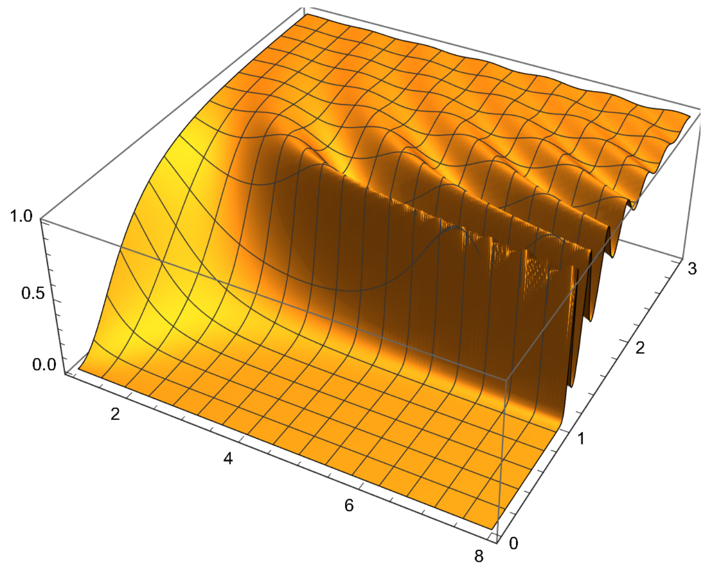
In[∘]:=
```
Plot[{tbar[k, 1], tbar[k, 2], tbar[k, 4]}, {k, 0, 4},
 AxesLabel → {"ka", "T"}, PlotLegends → {"La = 1", "La = 4", "La = 8"}]
```

Out[∘]=



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

Out[∘]=



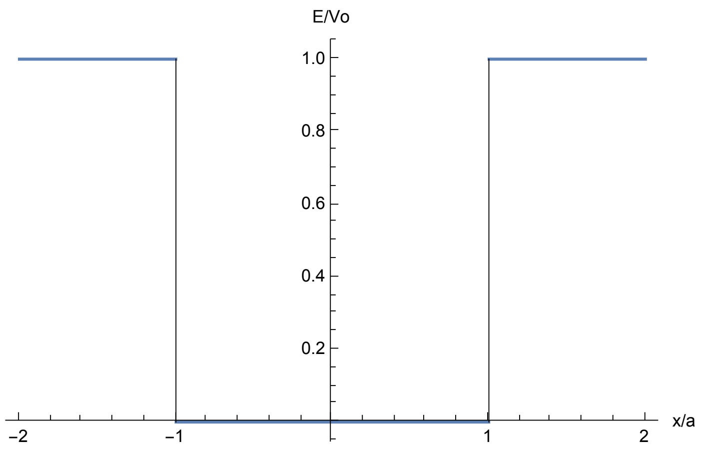
2.A.3. El pozo finito de potencial.

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}}]}]]
```

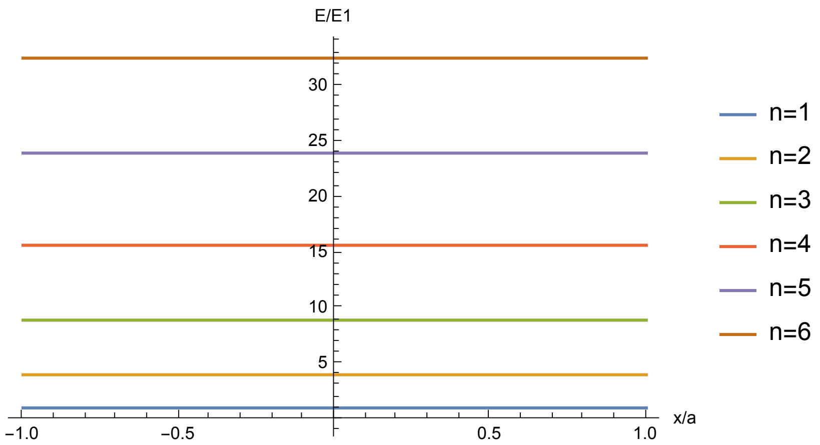
Out[∘]=



El espectro y las funciones propias para E < Vo.

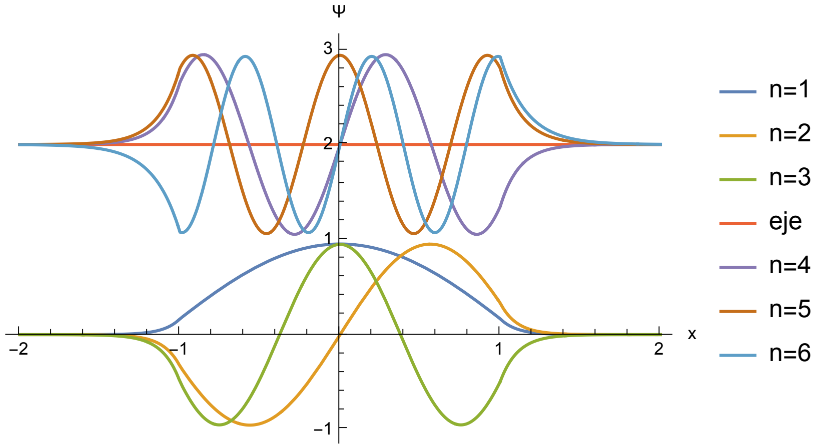
```
Plot[epozo, {x, -1, 1}, AxesLabel → {"x/a", "E/E1"},
 PlotLegends → {"n=1", "n=2", "n=3", "n=4", "n=5", "n=6"}]
```

Out[∘]=



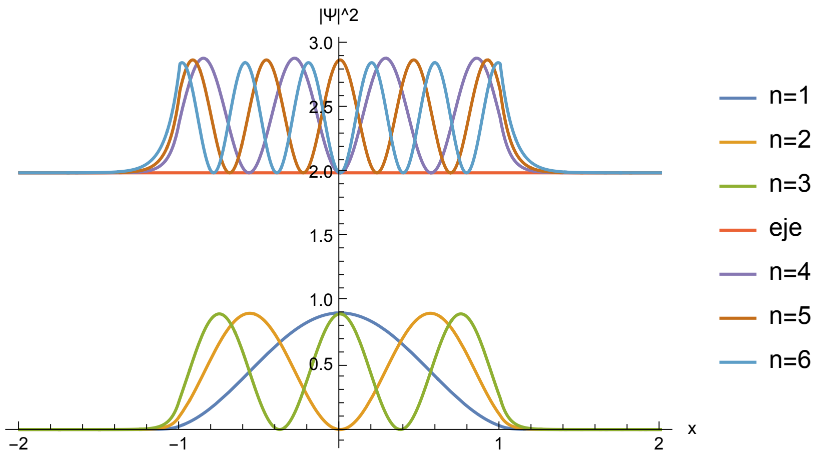
In[∘]:=
```
Plot[{fopozo⟦1⟧, fopozo⟦2⟧, fopozo⟦3⟧, 2, fopozo⟦4⟧ + 2,
  fopozo⟦5⟧ + 2, fopozo⟦6⟧ + 2}, {x, -2, 2}, AxesLabel → {"x", "Ψ"},
 PlotLegends → {"n=1", "n=2", "n=3", "eje", "n=4", "n=5", "n=6"}]
```

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"}]
```

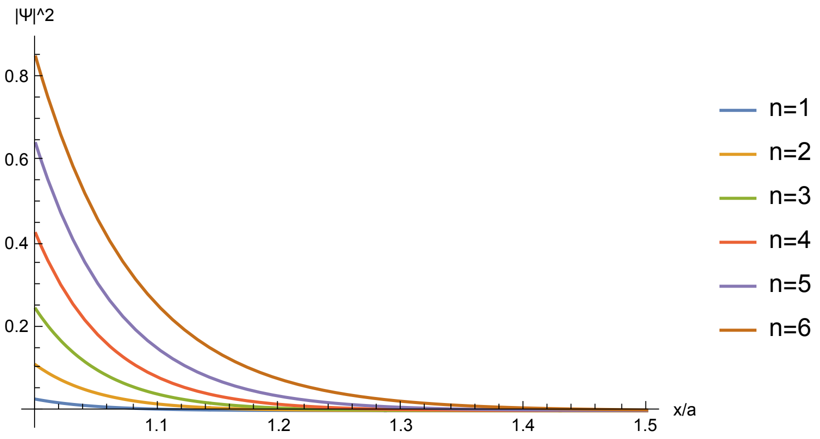
Out[∘]=



El efecto tunel cuando E < Vo.

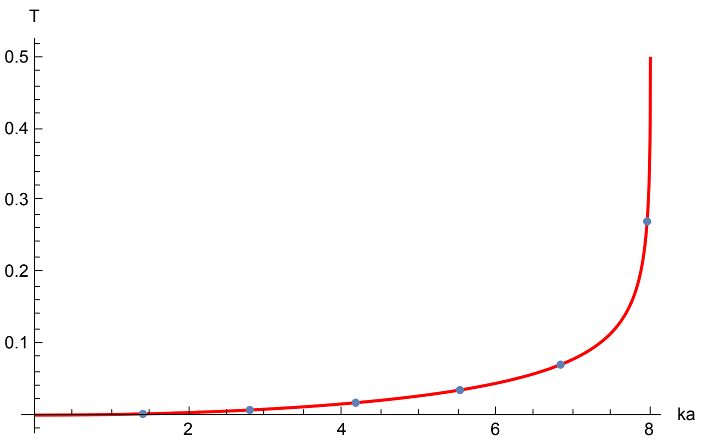
In[∘]:=
```
temp = Table[fopozo[[i]]^2, {i, nepozo}];
Plot[temp, {x, 1, 1.5}, PlotRange → All, AxesLabel → {"x/a", "|Ψ|^2"},
 PlotLegends → {"n=1", "n=2", "n=3", "n=4", "n=5", "n=6"}]
```

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[∘]=

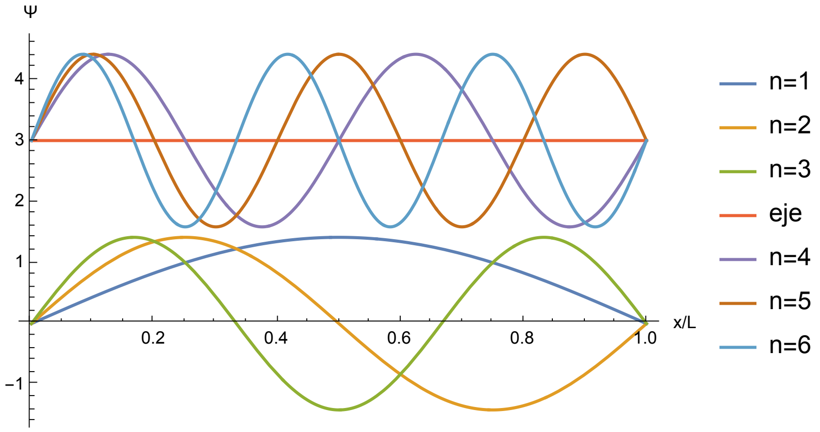


2.A.4. La partícula encerrada entre [0,L].

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"}]
```

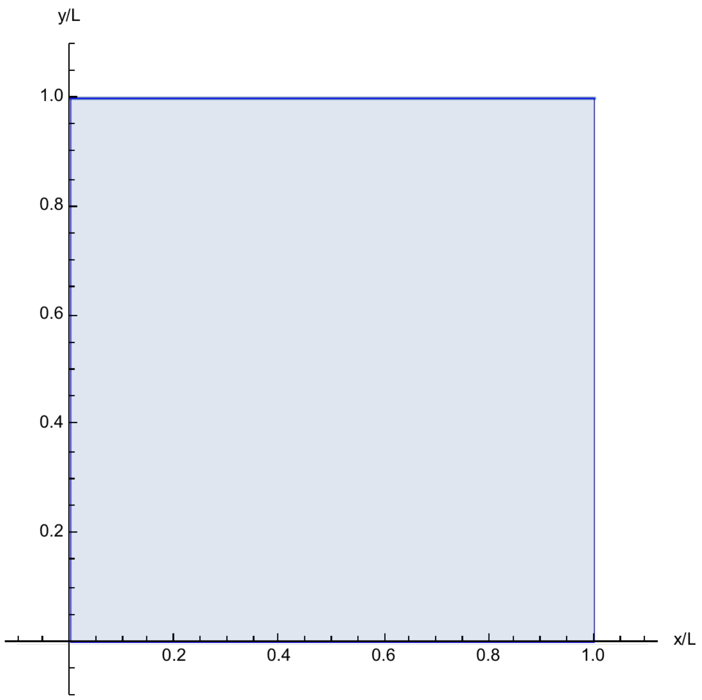
Out[∘]=



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}]}]
```

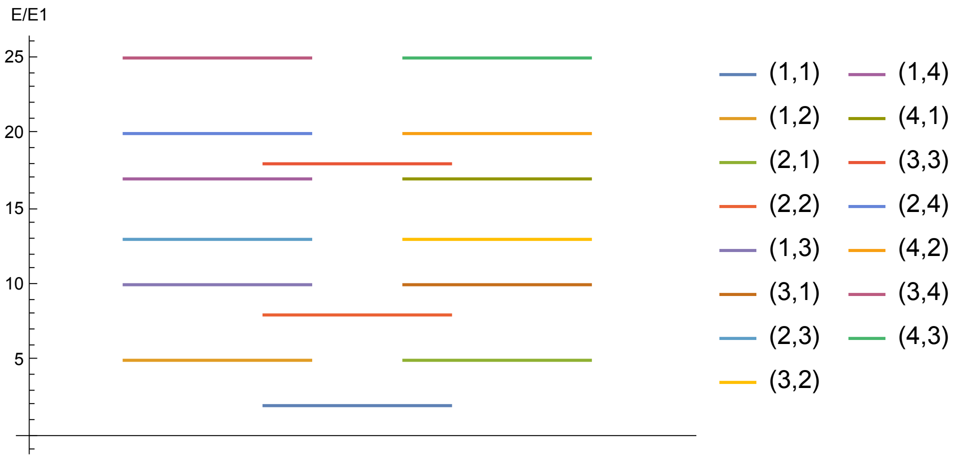
Energía, E(nx,ny):

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

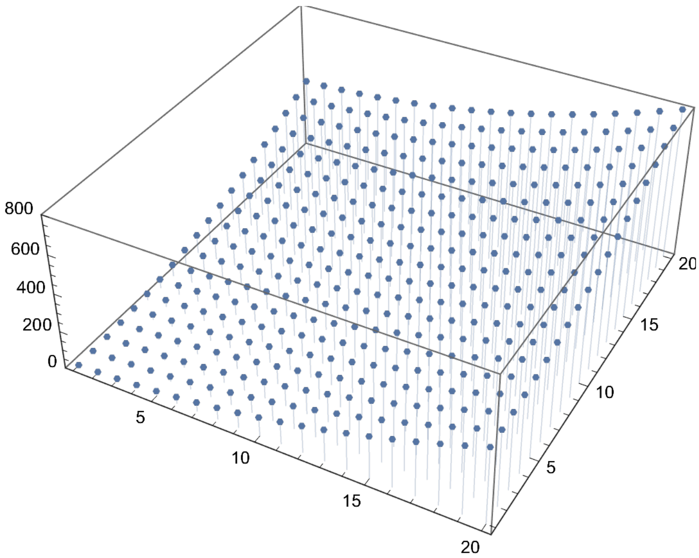
In[∘]:=
```
Plot[{edo[x, 2, 1.25], edo[x, 5, 0.5], edo[x, 5, 2],
   edo[x, 8, 1.25], edo[x, 10, 0.5], edo[x, 10, 2], edo[x, 13, 0.5],
   edo[x, 13, 2], edo[x, 17, 0.5], edo[x, 17, 2], edo[x, 18, 1.25],
   edo[x, 20, 0.5], edo[x, 20, 2], edo[x, 25, 0.5], edo[x, 25, 2]},
 {x, 0, 3.5}, AxesLabel → "E/E1", 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]
```

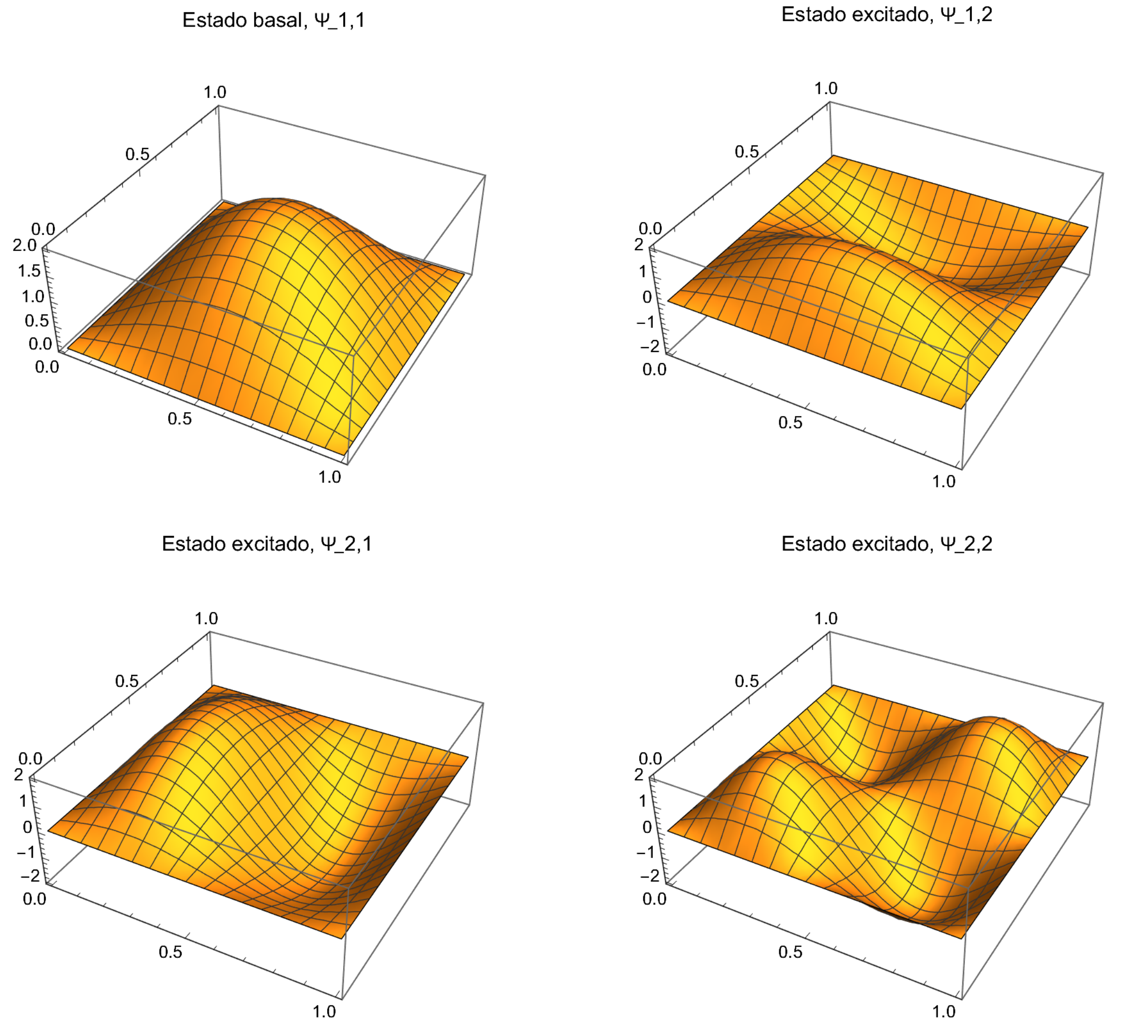
Out[∘]=



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"]}}]
```

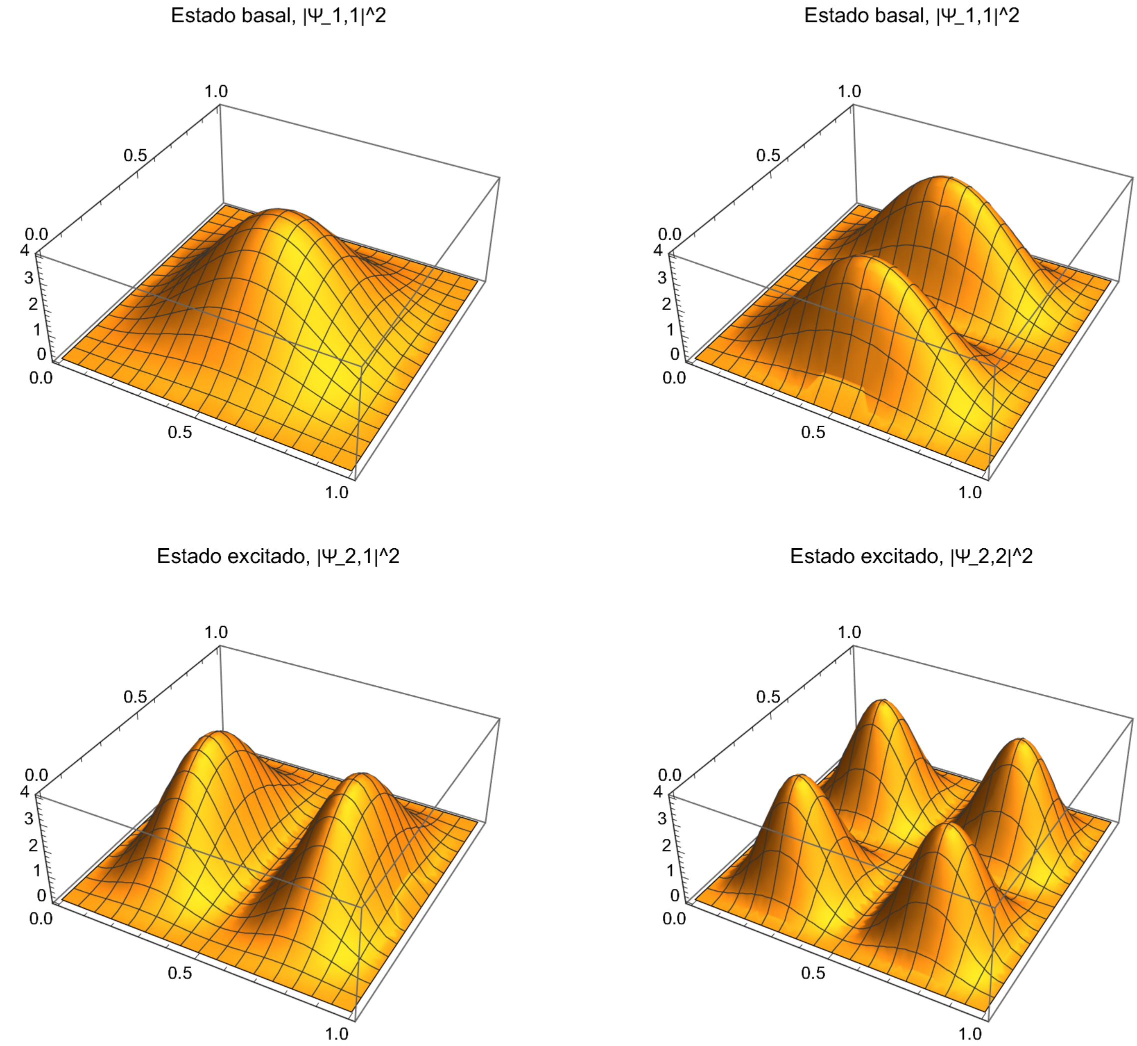
Out[ ]=



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.

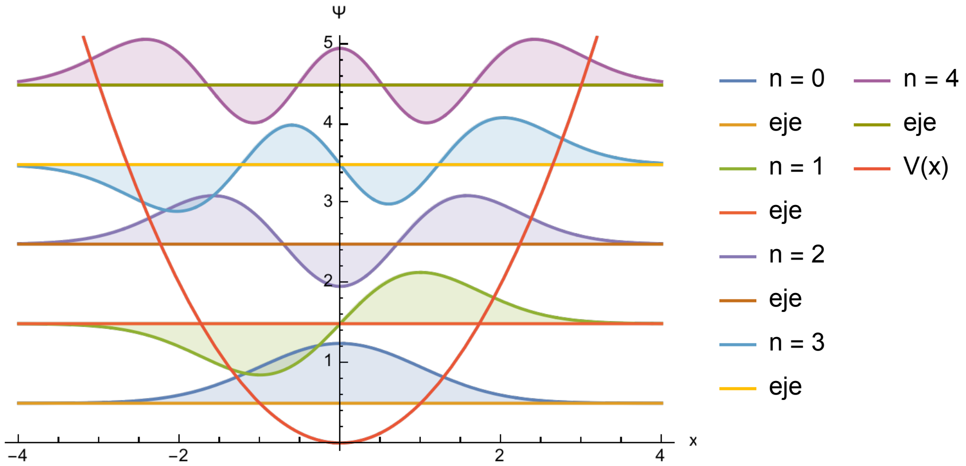
2.B.1. El oscilador armónico unidimensional.

Las funciones propias.

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

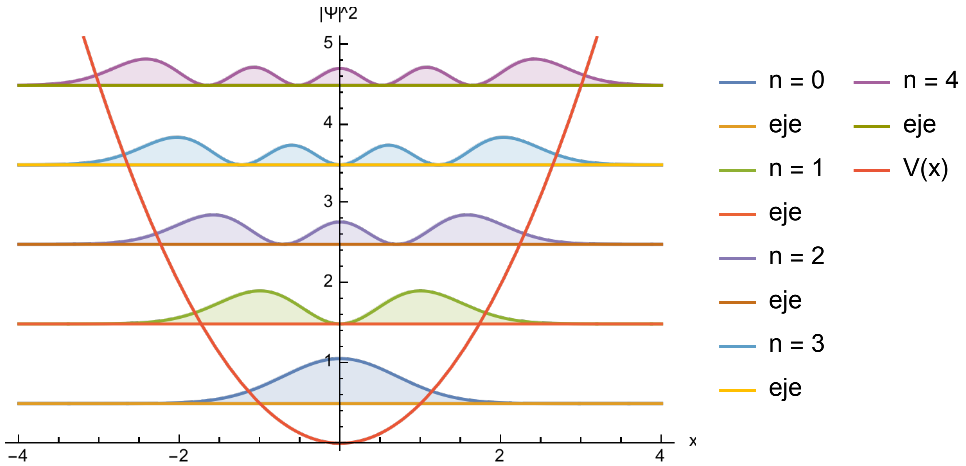
In[∘]:=
```
Plot[{0.5 + fooa[0, x], 0.5, 1.5 + fooa[1, x], 1.5, 2.5 + fooa[2, x], 2.5,
  3.5 + fooa[3, x], 3.5, 4.5 + fooa[4, x], 4.5, 0.5 * x * x}, {x, -4, 4},
 PlotLegends → {"n = 0", "eje", "n = 1", "eje", "n = 2", "eje",
   "n = 3", "eje", "n = 4", "eje", "V(x)"}, PlotRange → {-0.1, 5.1},
 Filling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

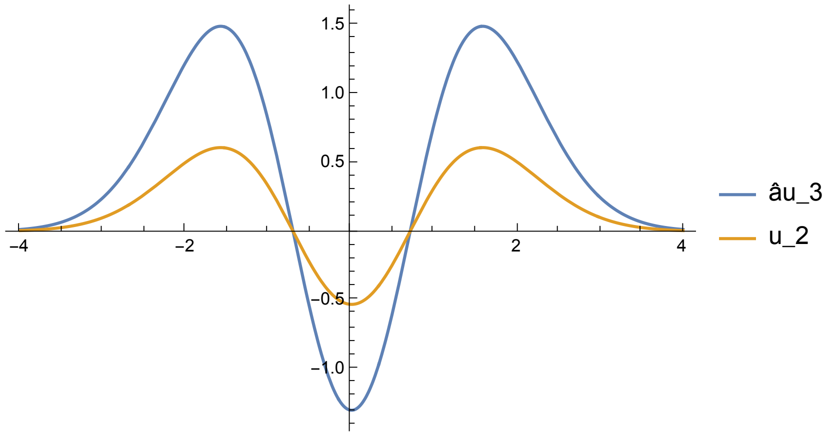
Out[∘]=



La acción de los operadores de ascenso y descenso.

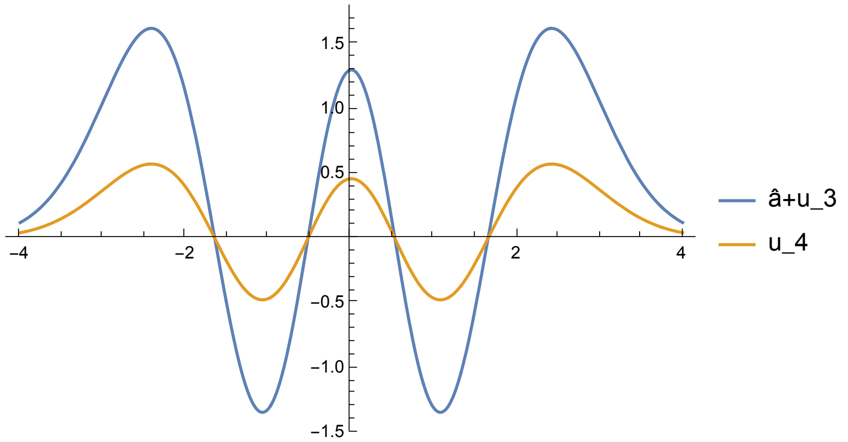
In[∘]:=
```
Plot[{x * fooa[3, x] + D[fooa[3, y], y] /. y → x, fooa[2, x]},
 {x, -4, 4}, PlotLegends → {"âu_3", "u_2"}]
```

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[∘]=



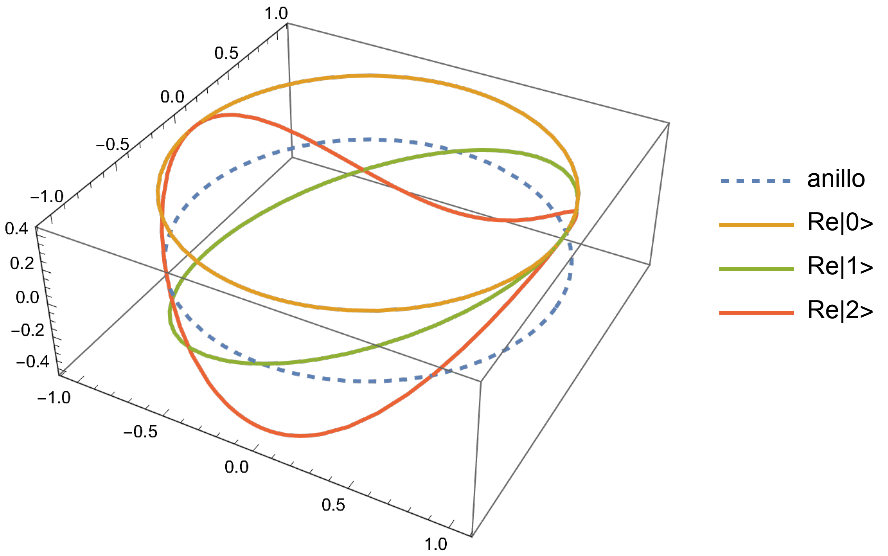
2.C. El movimiento rotacional.

2.C.1. La partícula en un anillo.

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

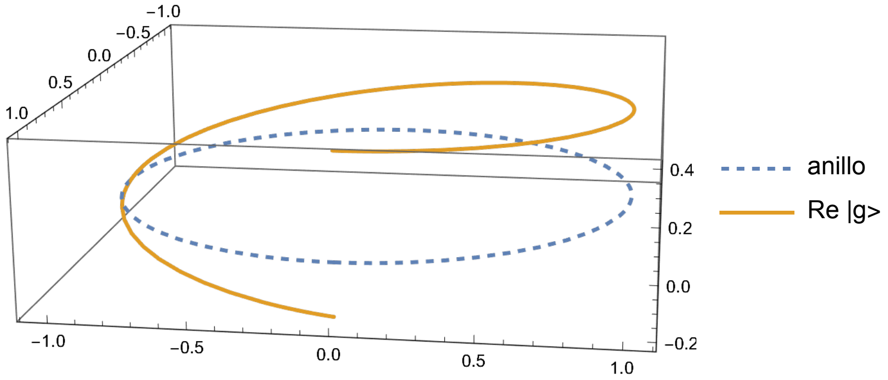
In[•]:=
```
ParametricPlot3D[{{Cos[a], Sin[a], 0}, {Cos[a], Sin[a], Re[fopan[0, a]]},
   {Cos[a], Sin[a], Re[fopan[1, a]]}, {Cos[a], Sin[a], Re[fopan[2, a]]}},
  {a, 0, 2 * Pi}, PlotStyle → { Dashed, Thick, Thick, Thick},
  PlotLegends → {"anillo", "Re|0>", "Re|1>", "Re|2>"}]
```

Out[•]=



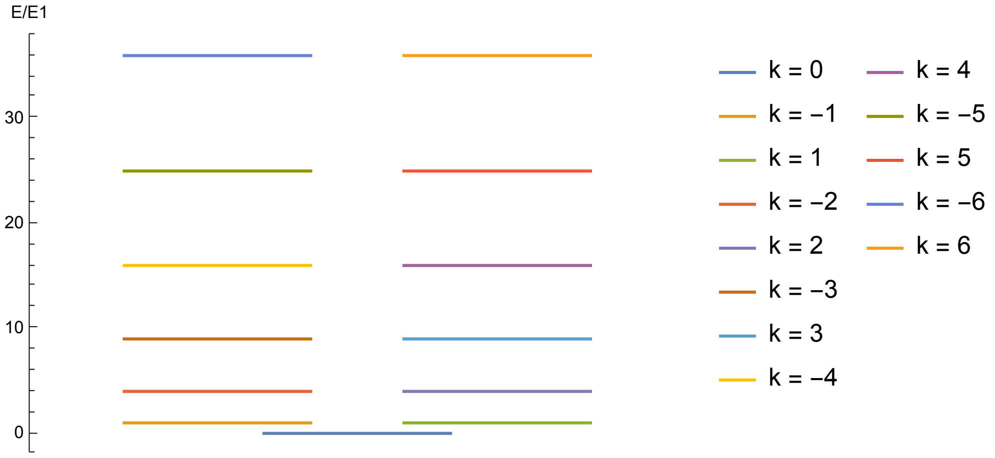
In[•]:=
```
ParametricPlot3D[{{Cos[a], Sin[a], 0}, {Cos[a], Sin[a], Re[fopan[1 / 3, a]]}},
  {a, 0, 2 * Pi}, PlotStyle → { Dashed, Thick, Thick, Thick},
  PlotLegends → {"anillo", "Re  |g>"}]
```

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[∘]=

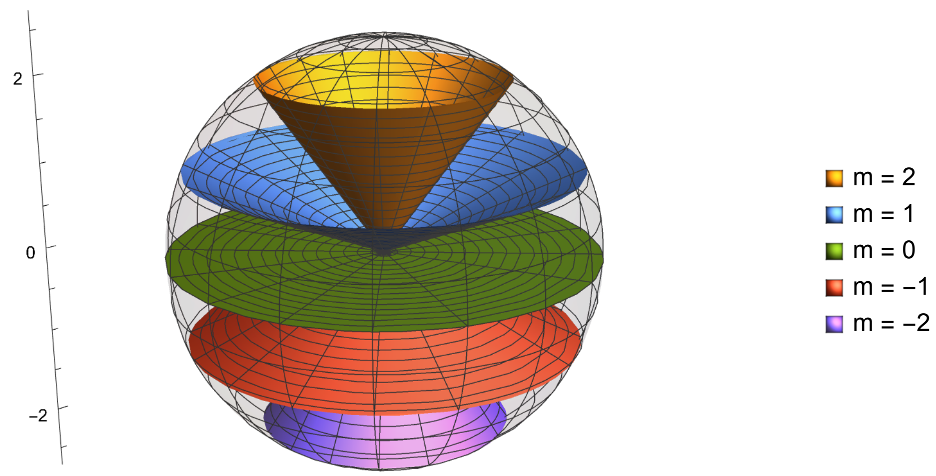


2.C.2. El momento angular.

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]
```

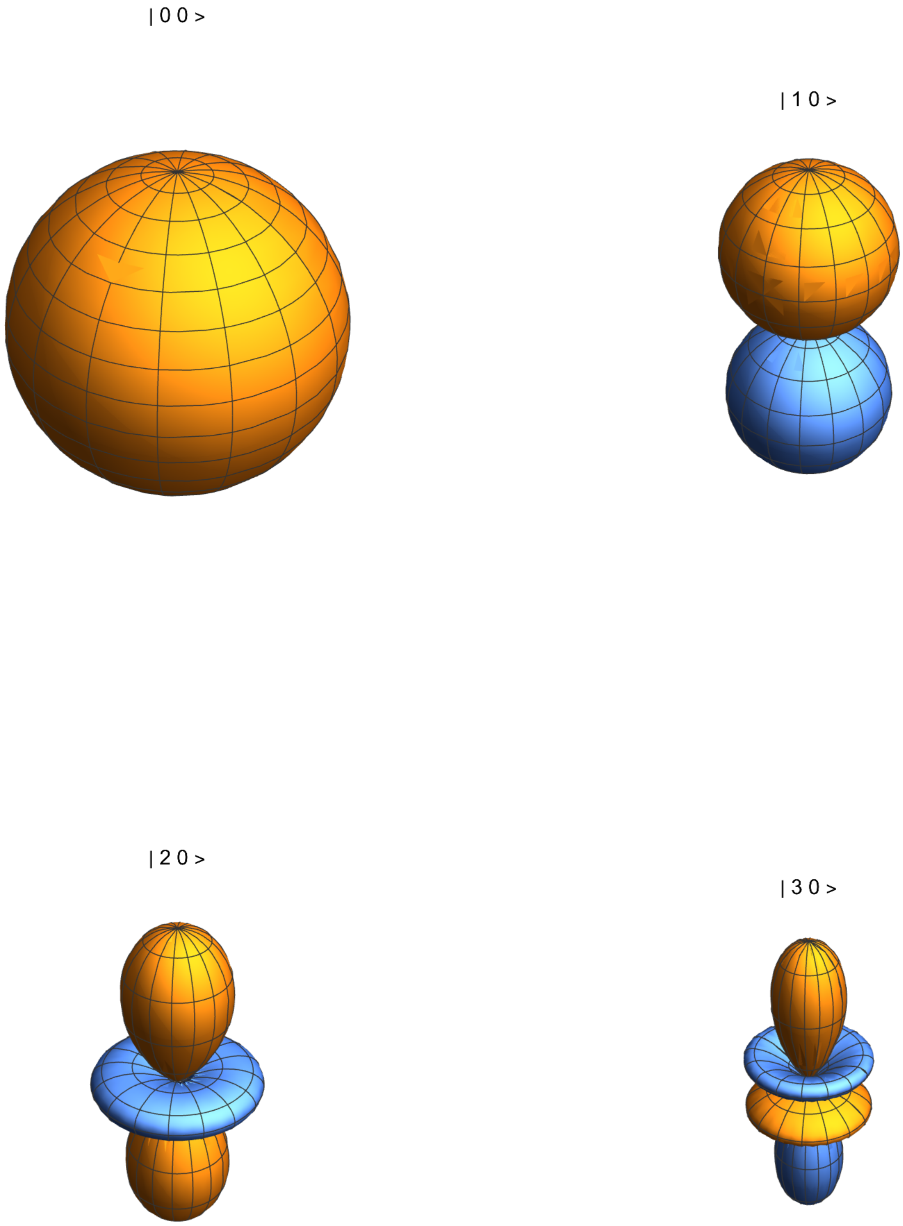
Out[∘]=



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]}}]
```

Out[ ]=

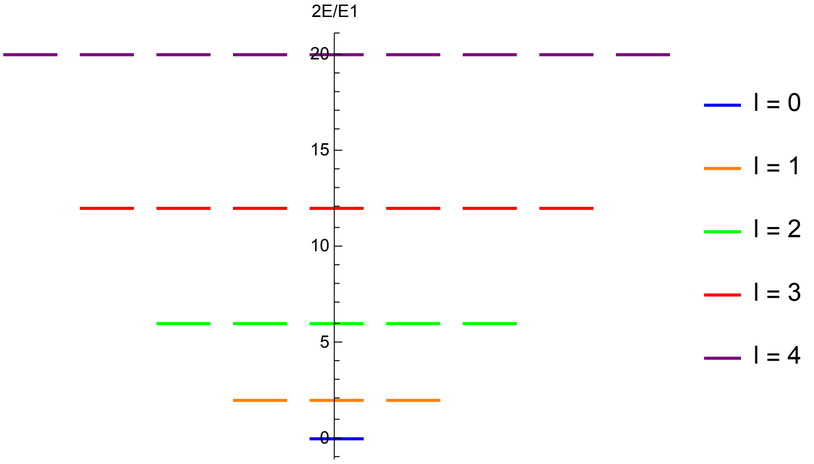


2.C.3. El rotor rígido.

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

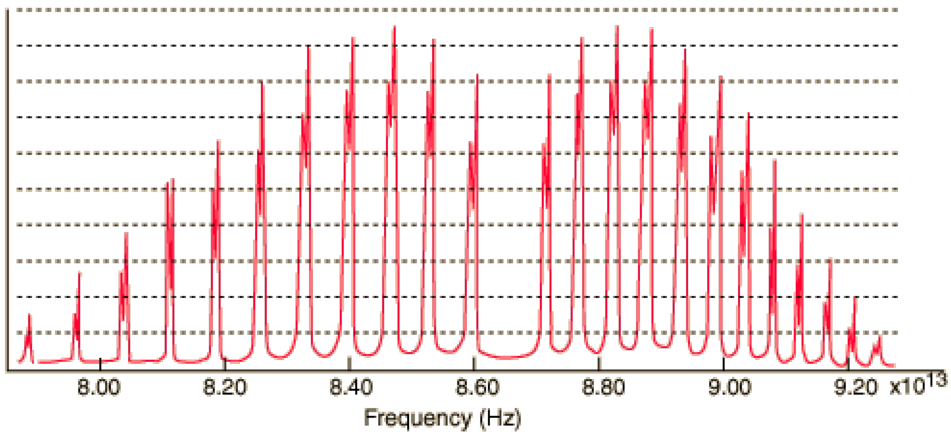
In[∘]:=
```
Show[Plot[Evaluate[edorr[0, y]], {y, -7, 7}, PlotRange → All, PlotStyle → Blue,
  PlotLegends → {"l = 0"}, Axes → {False, True}, AxesLabel → "2E/E1"],
 Plot[Evaluate[edorr[1, y]], {y, -7, 7}, PlotRange → All, PlotStyle → Orange,
  PlotLegends → {"l = 1"}], Plot[Evaluate[edorr[2, y]], {y,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



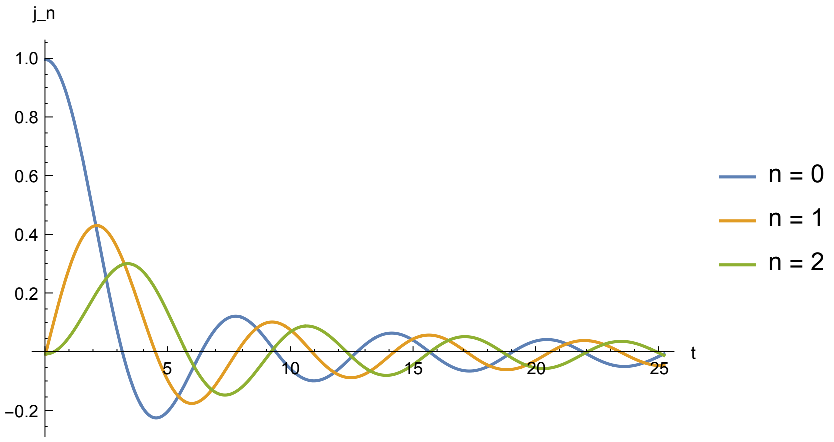
2.C.4. Los potenciales centrales: la partícula encerrada en una esfera.

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=

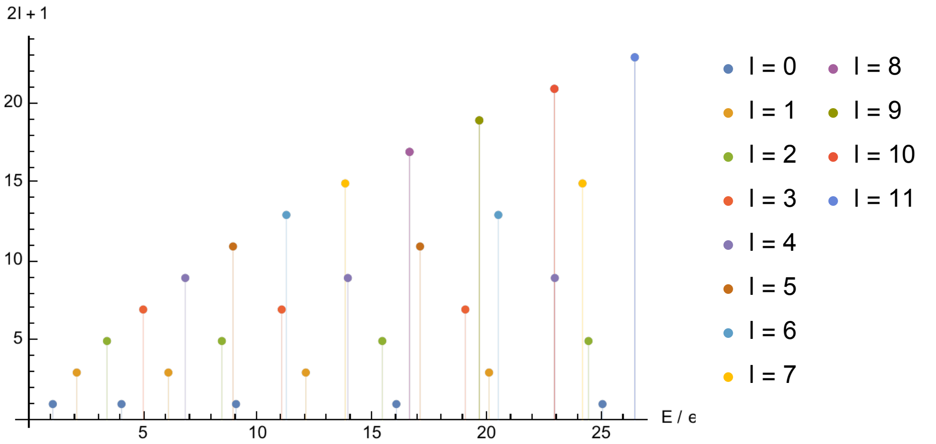
	j0	j1	j2	j3	j4	j5	j6
x1	3.14159	4.49341	5.76346	6.98793	8.18256	9.35581	10.5128
x2	6.28319	7.72525	9.09501	10.4171	11.7049	12.9665	14.2074
x3	9.42478	10.9041	12.3229	13.698	15.0397	16.3547	17.648
x4	12.5664	14.0662	15.5146	16.9236	18.3013	19.6532	20.9835
x5	15.708	17.2208	18.689	20.1218	21.5254	22.9046	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}]]
```

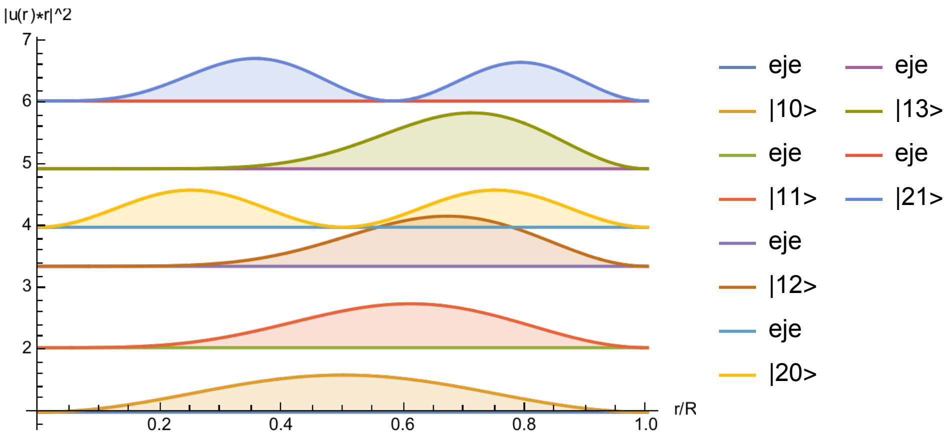
Out[∘]=



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

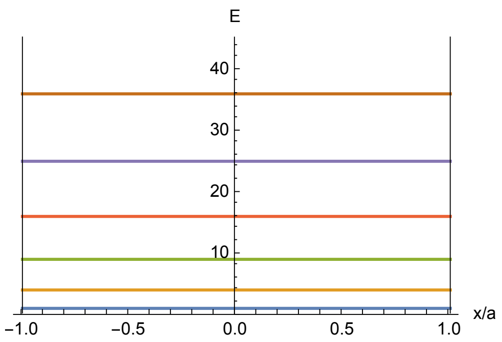
2.D. La teoría de perturbaciones.

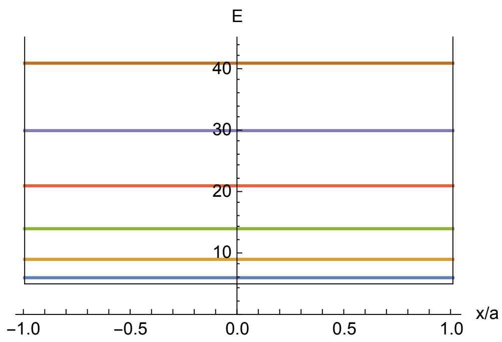
2.D.1. La teoría de perturbaciones independiente del tiempo.

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[∘]=

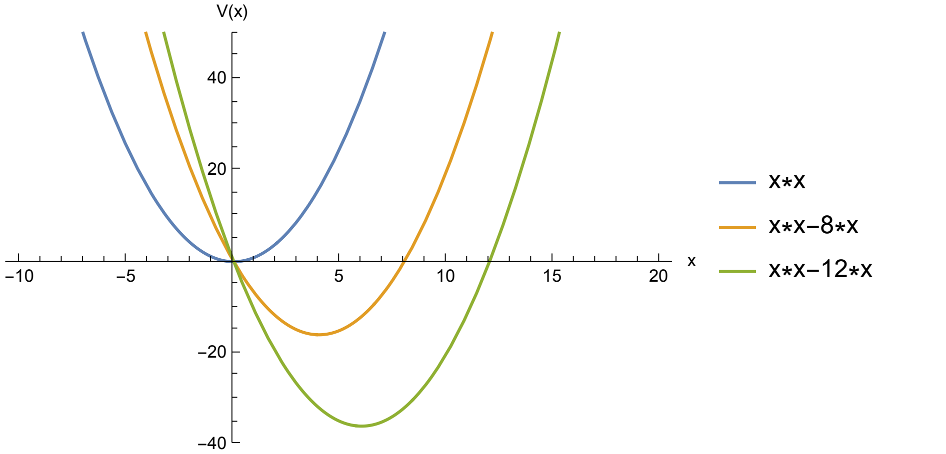




El oscilador armónico en presencia de una fuerza constante.

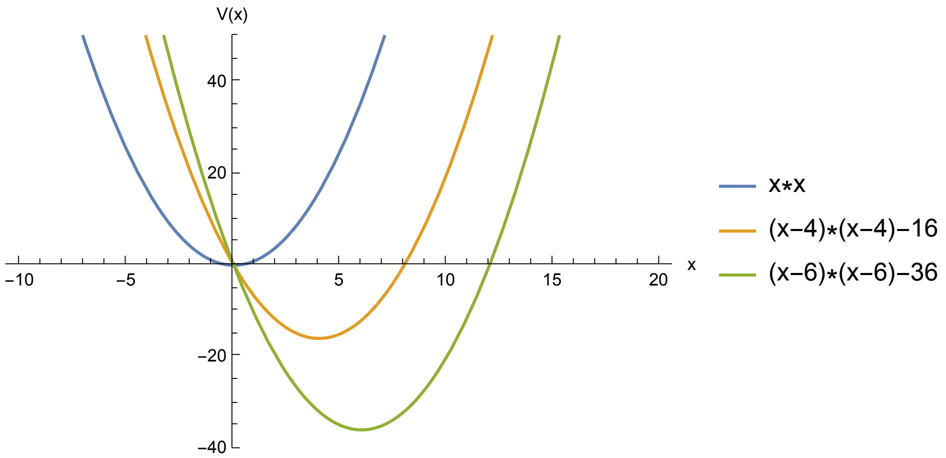
In[∘]:=
```
Plot[{x * x, x * x - 8 * x, x * x - 12 * x}, {x, -10, 20}, PlotRange → {-40, 50},
 AxesLabel → {"x", "V(x)"}, PlotLegends → {"x*x", "x*x-8*x", "x*x-12*x"}]
```

Out[∘]=



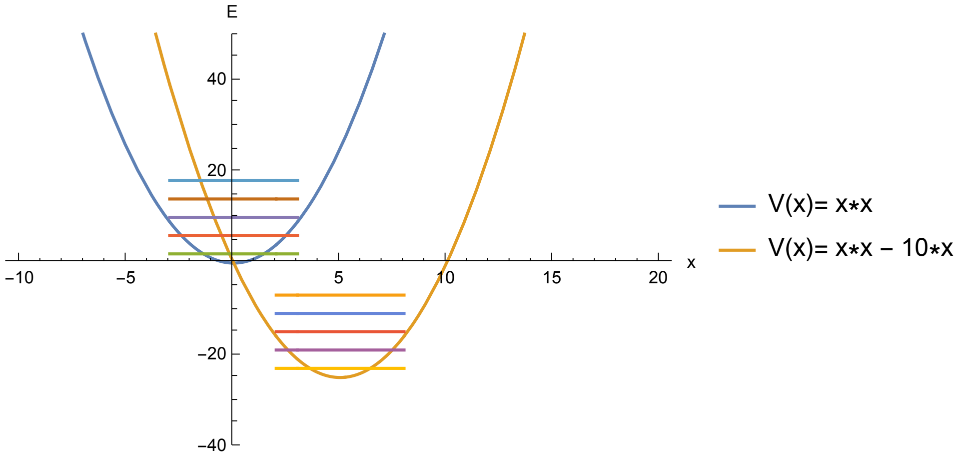
In[∘]:=
```
Plot[{x * x, (x - 4) * (x - 4) - 16, (x - 6) * (x - 6) - 36},
 {x, -10, 20}, PlotRange → {-40, 50}, AxesLabel → {"x", "V(x)"},
 PlotLegends → {"x*x", "(x-4)*(x-4)-16", "(x-6)*(x-6)-36"}]
```

Out[∘]=



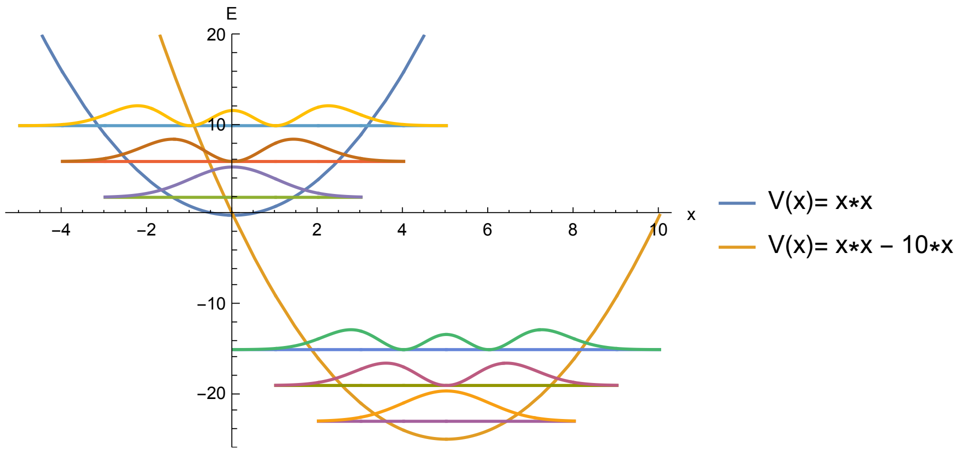
In[•]:=
```
Plot[{x * x, x * x - 10 * x, If[x > -3 && x < 3, 2],
  If[x > -3 && x < 3, 6], If[x > -3 && x < 3, 10], If[x > -3 && x < 3, 14],
  If[x > -3 && x < 3, 18], If[x > 2 && x < 8, -23], If[x > 2 && x < 8, -19], ,
  If[x > 2 && x < 8, -15], If[x > 2 && x < 8, -11], If[x > 2 && x < 8, -7]},
 {x,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

Out[•]=



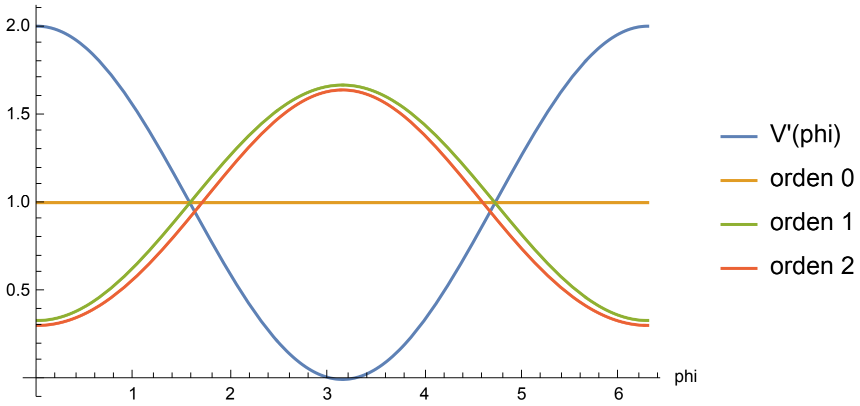
In[•]:=
```
Plot[{x * x, x * x - 10 * x, If[x > -3 && x < 3, 2],
  If[x > -4 && x < 4, 6], If[x > -3 && x < 3, 6 * fooa[0, x / Sqrt[2]] ^2 + 2],
  If[x > -4 && x < 4, 6 * fooa[1, x / Sqrt[2]] ^2 + 6], If[x > -5 && x < 5, 10],
  If[x > -5 && x < 5, 6 * fooa[2, x / Sqrt[2]] ^2 + 10],
  If[x > 2 && x < 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[•]=

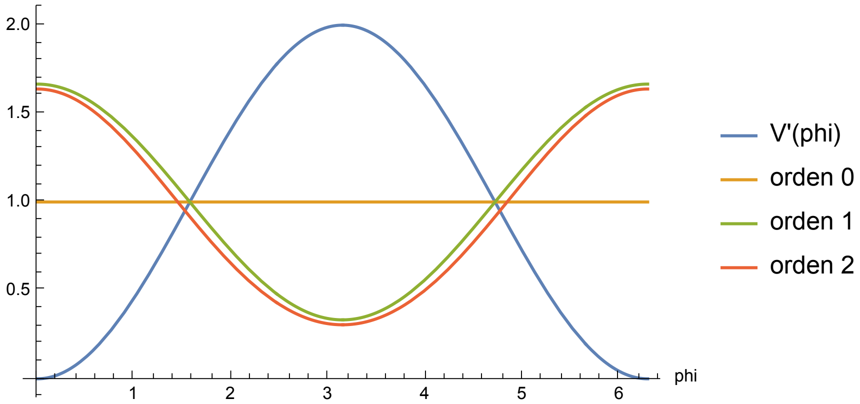


La partícula en un anillo con un potencial cosenoidal.

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"}]
```

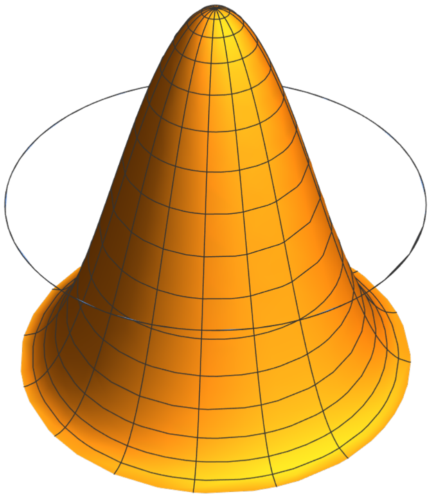
Out[∘]=


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=

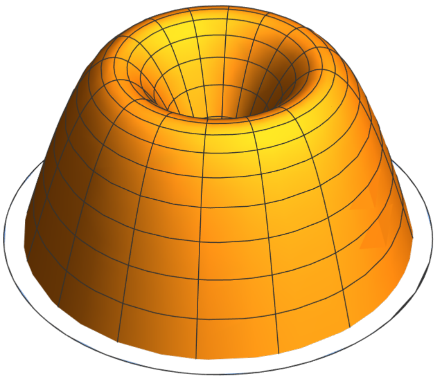
	l=0	l=1	l=2	l=3	l=4
n=1	-7.58942×10^{-16}	-0.254408	-0.409114	-0.513051	-0.587558
n=2	7.37257×10^{-17}	-0.0824195	-0.170607	-0.250223	-0.319288
n=3	0.	-0.04094	-0.0939641	-0.148635	-0.201009
n=4	-2.94903×10^{-17}	-0.024501	-0.0595651	-0.0985984	-0.138351
n=5	-3.46945×10^{-18}	-0.0163133	-0.0411527	-0.0702286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

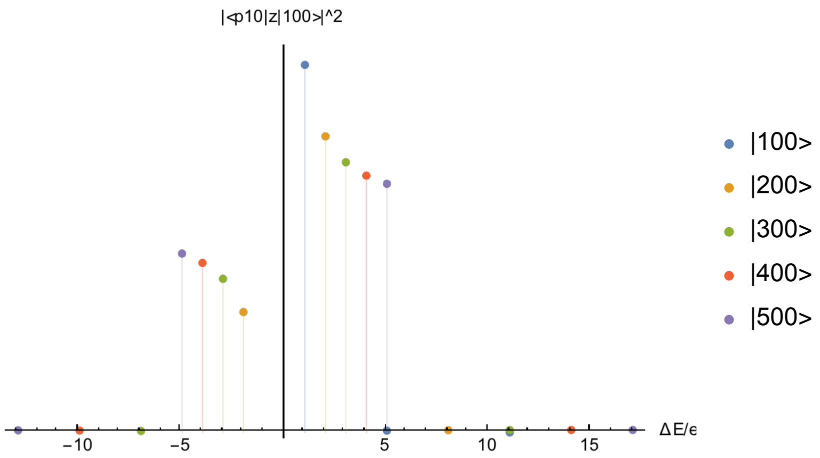
Out[∘]//TableForm=

	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.

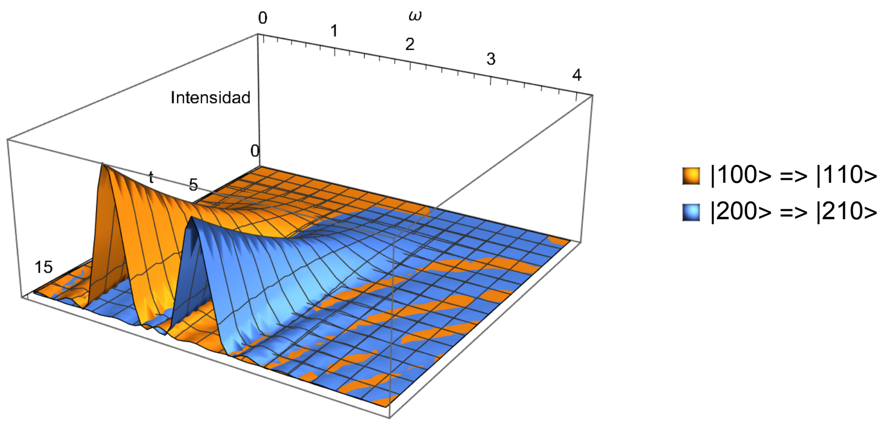
In[∘]:=
```
temp = Table[{(zsb[1, p]^2 - zsb[0, 1]^2) / Pi^2,
    NIntegrate[radps[p, 1, t] * radps[1, 0, t] * t^3, {t, 0, 1}]^2}, {p, 3}];
temp = Append[{temp}, Table[{(zsb[1, p]^2 - zsb[0, 2]^2) / Pi^2,
     NIntegrate[radps[p, 1, t] * radps[2, 0, t] * t^3, {t, 0, 1}]^2}, {p, 3}]];
temp = Append[temp, 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.

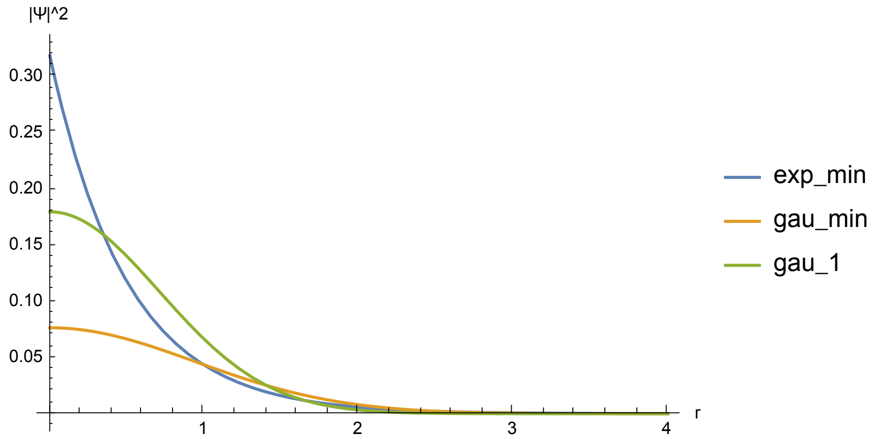
3.A. Los átomos hidrogenoides.

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];
```

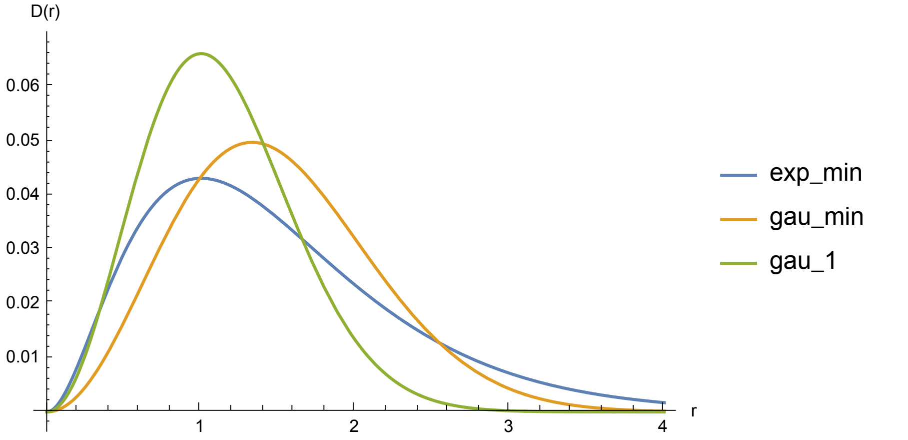
In[∘]:=
```
Plot[{prexp[1, r], prgau[4 / (3 * Sqrt[Pi]), r], prgau[1, r]},
 {r, 0, 4}, PlotRange → All, AxesLabel → {"r", "|Ψ|^2"},
 PlotLegends → {"exp_min", "gau_min", "gau_1"}]
```

Out[∘]=



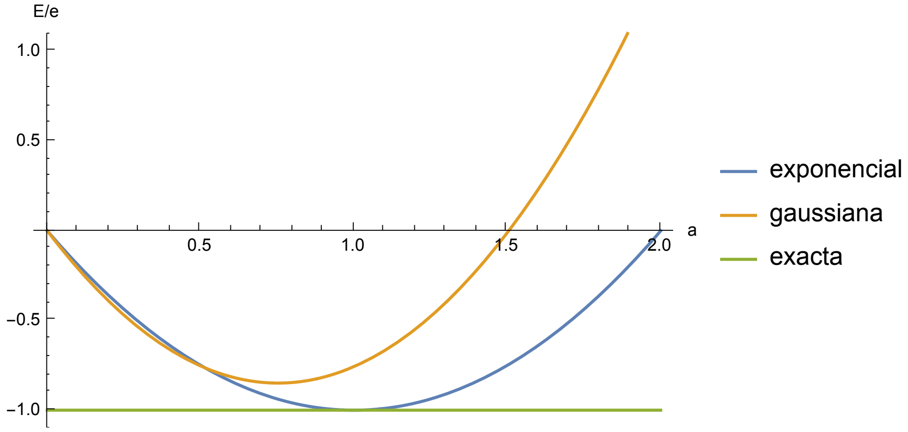
In[∘]:=
```
Plot[{prexp[1, r] * r * r, prgau[4 / (3 * Sqrt[Pi]), r] * r * r, prgau[1, r] * r * r},
  {r, 0, 4}, PlotRange → All, AxesLabel → {"r", "D(r)"},
  PlotLegends → {"exp_min", "gau_min", "gau_1"}]
```

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"}]
```

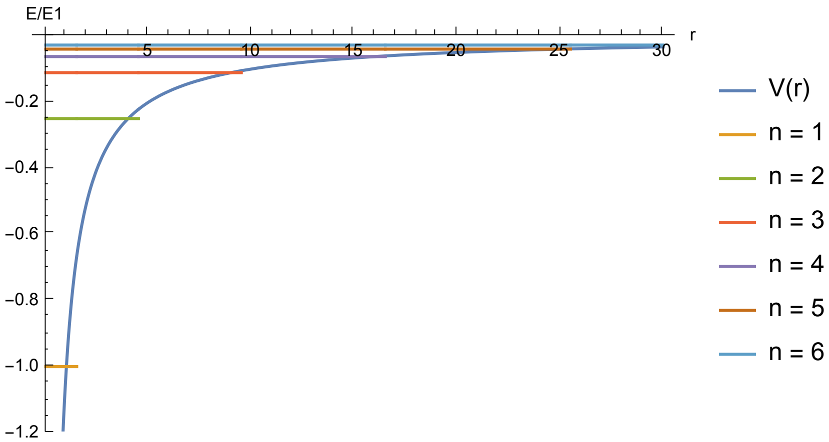
Out[∘]=



3.A.2. El espectro.

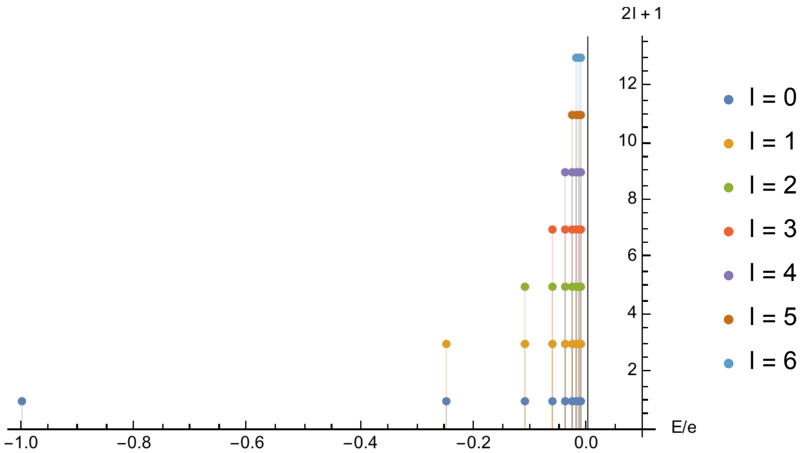
In[∘]:=
```
Plot[{-1 / r, If[r < 1 + 0.5, - 1], If[r < 4 + 0.5, - 1 / 4], If[r < 9 + 0.5, - 1 / 9],
  If[r < 16 + 0.5, - 1 / 16], If[r < 25 + 0.5, - 1 / 25], If[r < 36 + 0.5, - 1 / 36]},
 {r, 0, 30}, PlotRange → {-1.2, 0}, AxesLabel → {"r", "E/E1"},
 PlotLegends → Join[{"V(r)"}, Table["n = " <> ToString[n],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



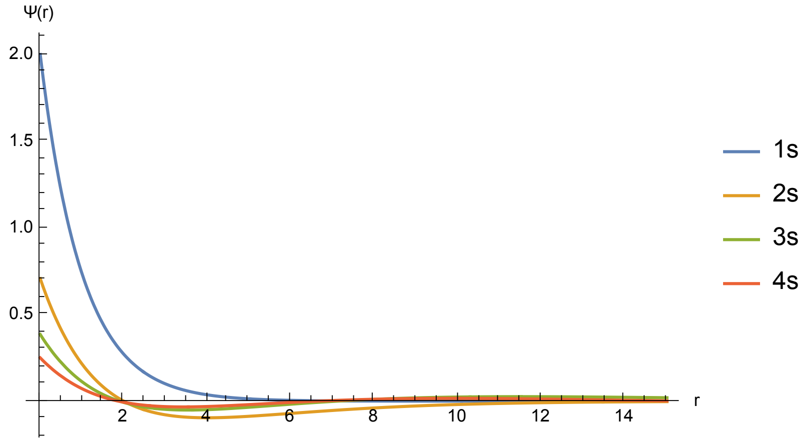
3.A.3. Las funciones de onda y las distribuciones radiales.

Las funciones.

Los orbitales tipo s.

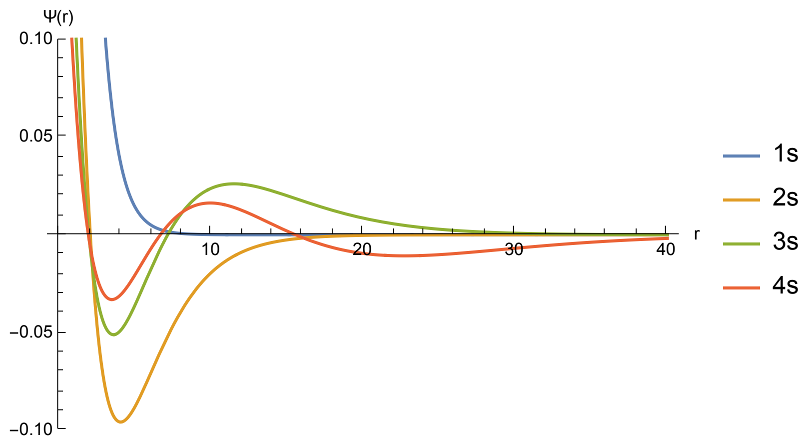
In[∘]:=
```
Plot[{radhid[1, 0, r] * nohid[1, 0], radhid[2, 0, r] * nohid[2, 0],
   radhid[3, 0, r] * nohid[3, 0], radhid[4, 0, r] * nohid[4, 0]},
 {r, 0, 15}, PlotRange → All, PlotLegends → {"1s", "2s", "3s", "4s"},
 AxesLabel → {"r", "Ψ(r)"}]
```

Out[∘]=



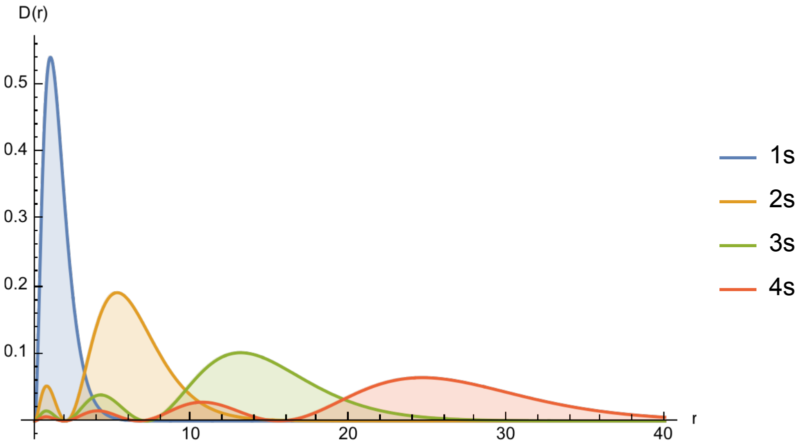
In[∘]:=
```
Plot[{radhid[1, 0, r] * nohid[1, 0], radhid[2, 0, r] * nohid[2, 0],
   radhid[3, 0, r] * nohid[3, 0], radhid[4, 0, r] * nohid[4, 0]}, {r, 0, 40},
 PlotRange → {-0.1, 0.1}, PlotLegends → {"1s", "2s", "3s", "4s"},
 AxesLabel → {"r", "Ψ(r)"}]
```

Out[∘]=



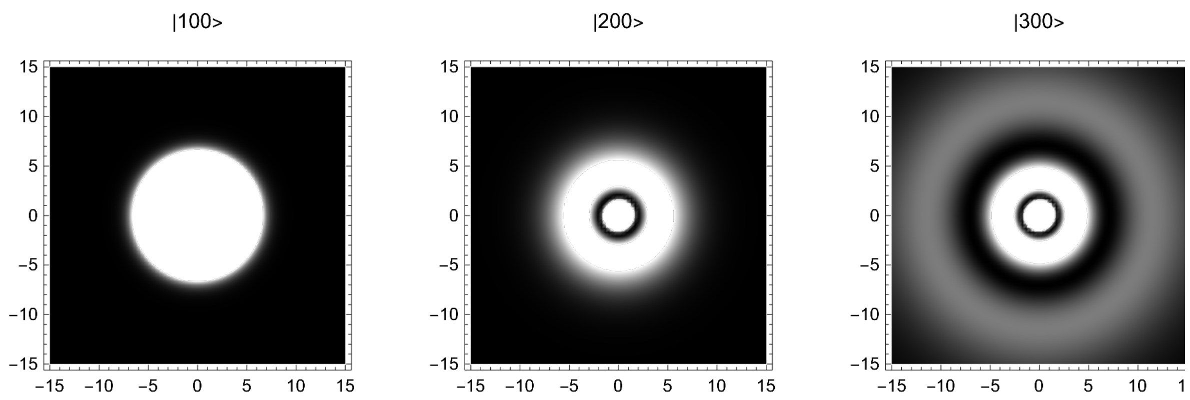
In[∘]:=
```
Plot[{(radhid[1, 0, r] * r * nohid[1, 0]) ^2, (radhid[2, 0, r] * r * nohid[2, 0]) ^2,
   (radhid[3, 0, r] * r * nohid[3, 0]) ^2, (radhid[4, 0, r] * r * nohid[4, 0]) ^2},
  {r, 0, 40}, PlotRange → All, PlotLegends → {"1s", "2s", "3s", "4s"},
  AxesLabel → {"r", "D(r)"}, Filling → Axis]
```

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>"]}}]
```

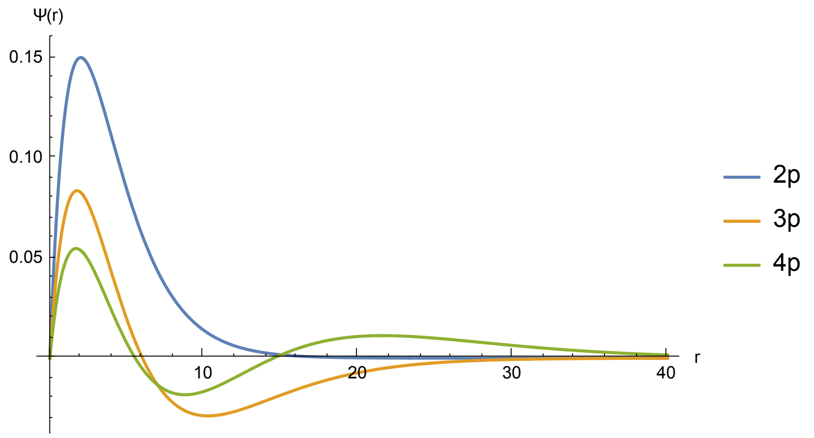
Out[∘]=



Los orbitales tipo p.

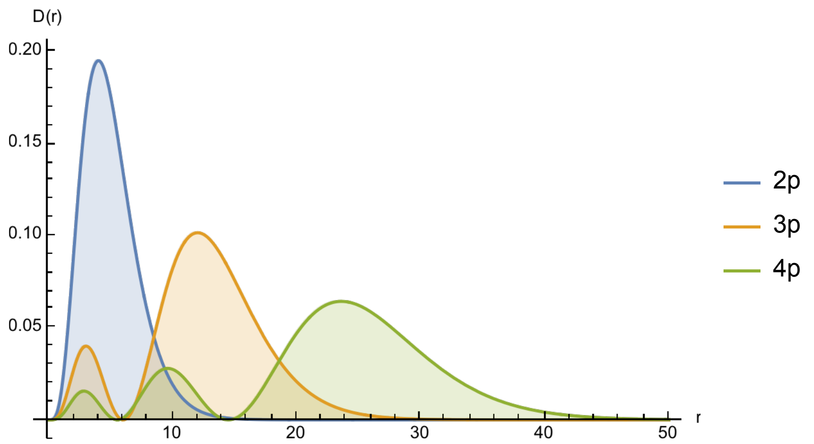
In[∘]:=
```
Plot[{radhid[2, 1, r] * nohid[2, 1], radhid[3, 1, r] * nohid[3, 1],
  radhid[4, 1, r] * nohid[4, 1]}, {r, 0, 40}, PlotRange → All,
 PlotLegends → {"2p", "3p", "4p"}, AxesLabel → {"r", "Ψ(r)"}]
```

Out[∘]=



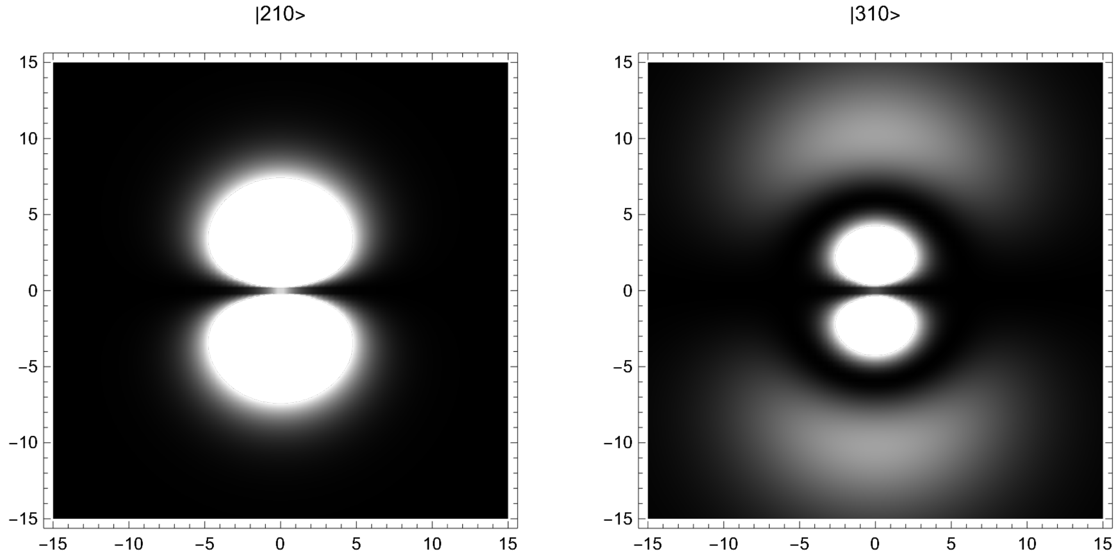
In[∘]:=
```
Plot[{(radhid[2, 1, r] * r * nohid[2, 1]) ^2, (radhid[3, 1, r] * r * nohid[3, 1]) ^2,
  (radhid[4, 1, r] * r * nohid[4, 1]) ^2}, {r, 0, 50}, PlotRange → All,
 PlotLegends → {"2p", "3p", "4p"}, AxesLabel → {"r", "D(r)"}, Filling → Axis]
```

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>"]}}]
```

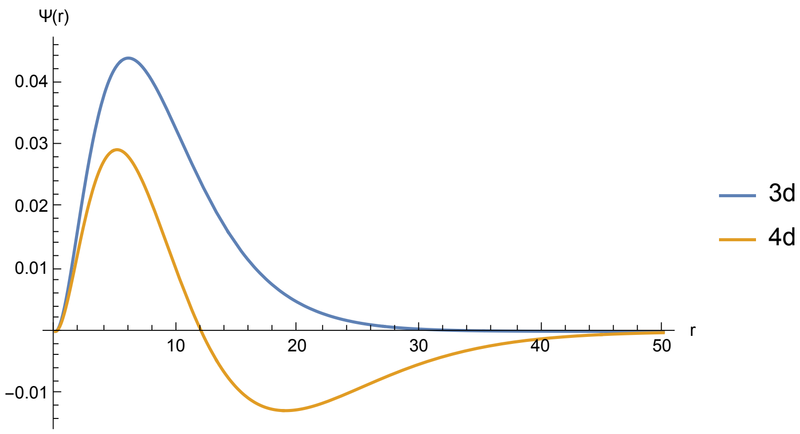
Out[∘]=



Los orbitales tipo d.

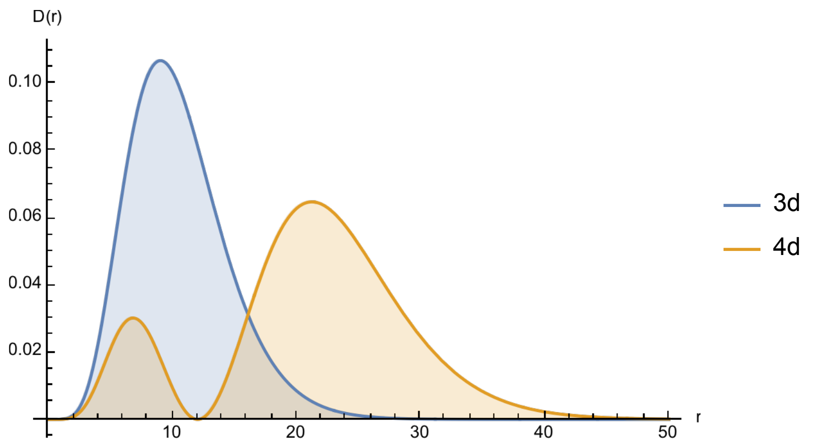
In[∘]:=
```
Plot[{radhid[3, 2, r] * nohid[3, 2], radhid[4, 2, r] * nohid[4, 2]}, {r, 0, 50},
 PlotRange → All, PlotLegends → {"3d", "4d"}, AxesLabel → {"r", "Ψ(r)"}]
```

Out[∘]=



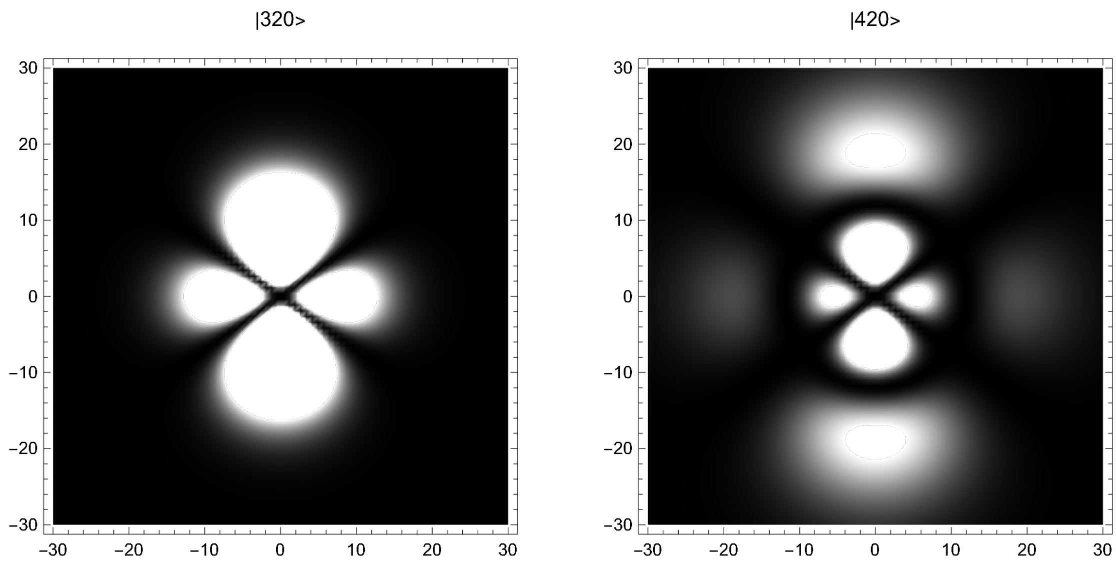
In[ ]:=
```
Plot[{(radhid[3, 2, r] * r * nohid[3, 2]) ^2, (radhid[4, 2, r] * r * nohid[4, 2]) ^2},
 {r, 0, 50}, PlotRange → All, PlotLegends → {"3d", "4d"},
 AxesLabel → {"r", "D(r)"}, Filling → Axis]
```

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>"]}}]
```

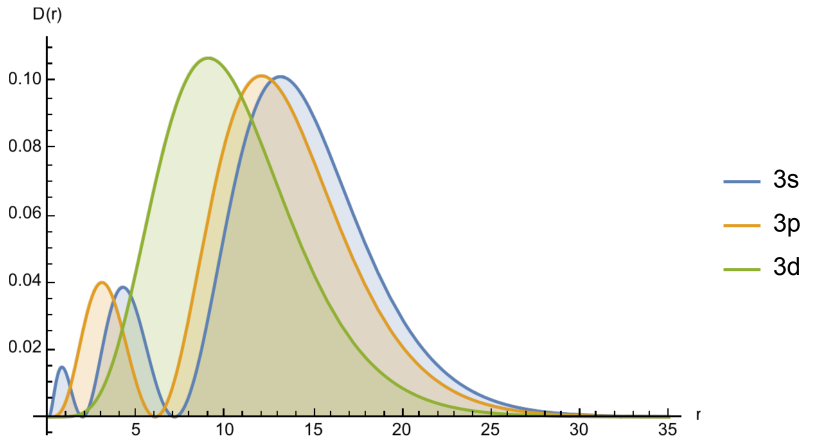
Out[ ]=



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=
```
           r → 13.074
           r → 7.09808
l = 0      r → 4.18593
           r → 1.90192
           r → 0.740037
           r → 12.
l = 1      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
```

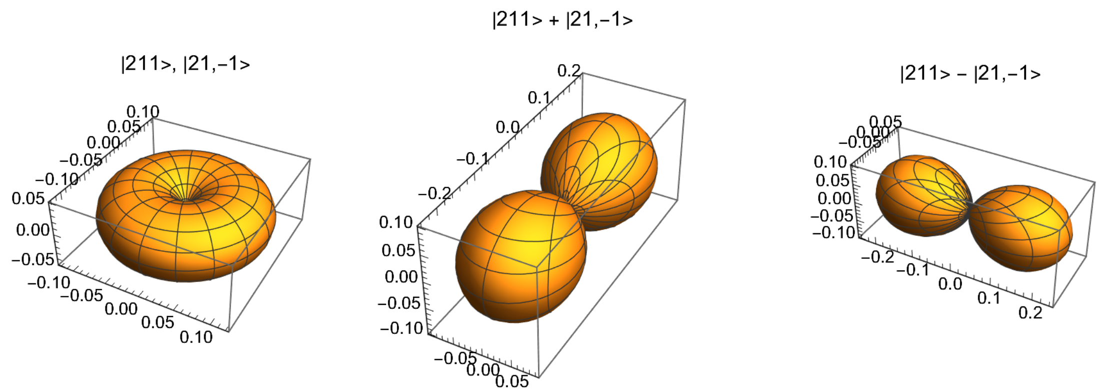
```
Nodos:
```

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}]}]
```

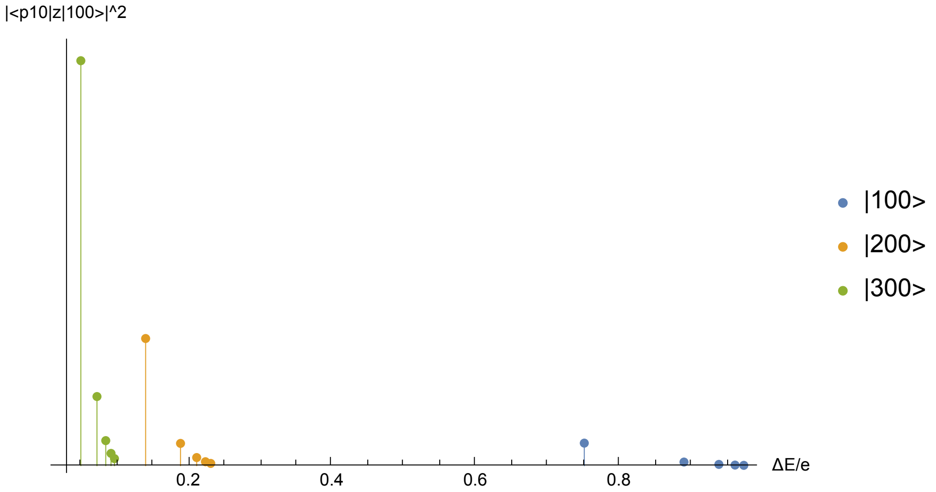
Out[∘]//TableForm=

	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.

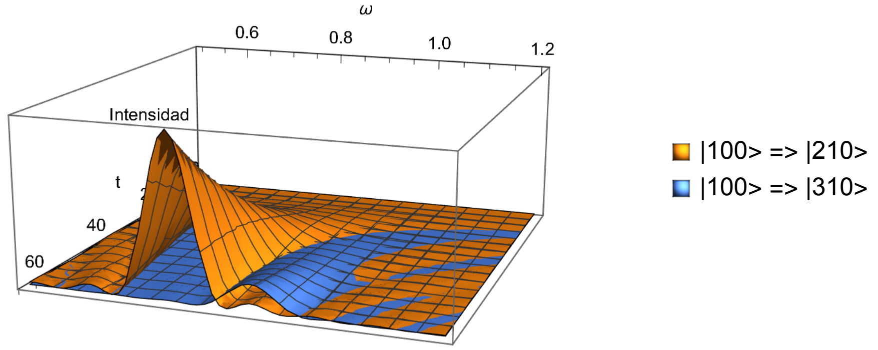
In[∘]:=
```
temp = Table[{1 - 1 / p^2, (nohid[p, 1] * nohid[1, 0] * NIntegrate[
        radhid[p, 1, t] * radhid[1, 0, t] * t^3, {t, 0, Infinity}]) ^2}, {p, 2, 6}];
temp = Append[{temp},
   Table[{1 / 4 - 1 / p^2, (nohid[p, 1] * nohid[2, 0] * NIntegrate[radhid[p, 1, t] *
          radhid[2, 0, t] * t^3, {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[∘]=

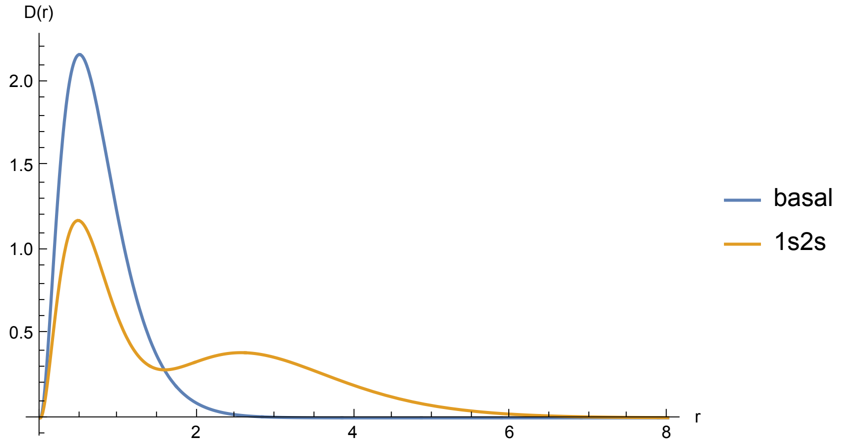


3.B. El átomo de helio.

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"}]
```

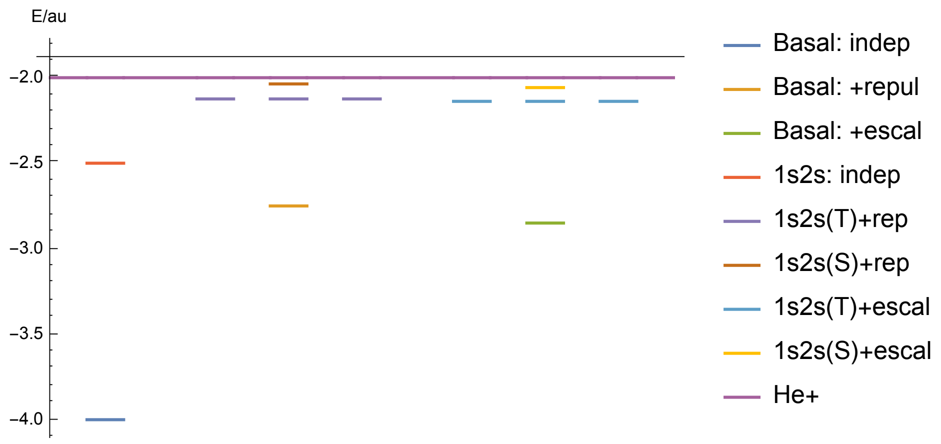
Out[◦]=



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

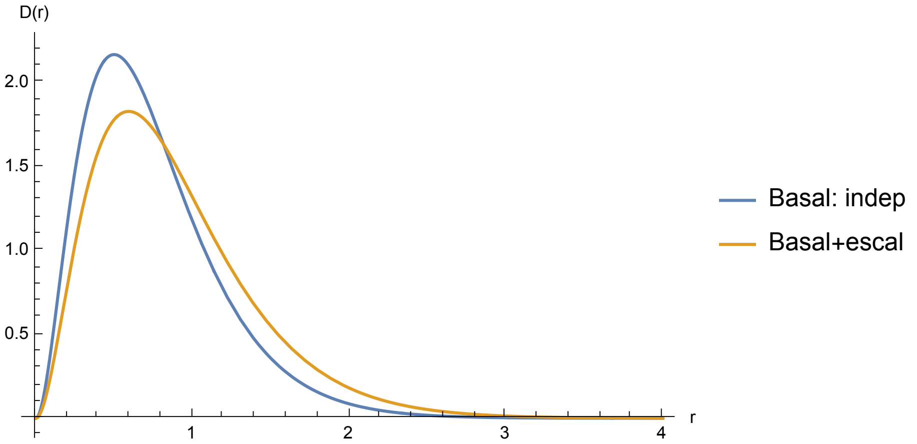
In[◦]:=
```
Plot[{If[x > 1 && x < 2, -4], If[x > 6 && x < 7, -2.75],
  If[x > 13 && x < 14, -2.85], If[x > 1 && x < 2, -2.5],
  If[x > 4 && x < 5 || x > 6 && x < 7 || x > 8 && x < 9, -2.5 + 34 / 81 - 32 / 729],
  If[x > 6 && x < 7, -2.5 + 34 / 81 + 32 / 729],
  If[x > 11 && x < 12 || x > 13 && x < 14 || 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[◦]=

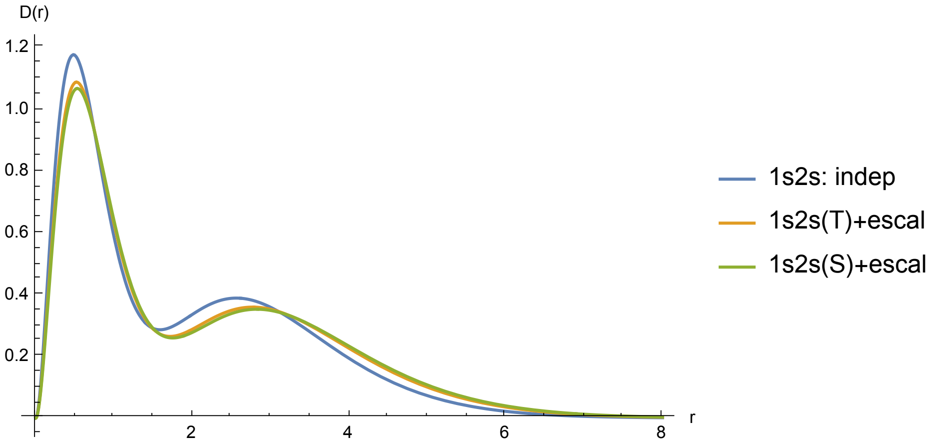


3.B.3. Las funciones de onda escaladas.

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.

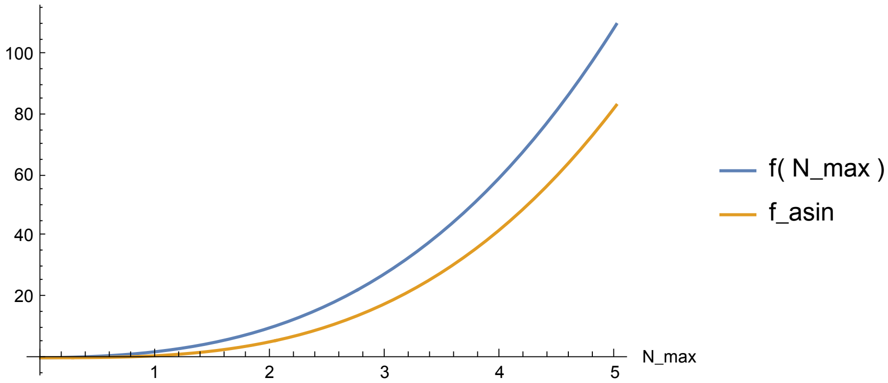
3.C.1. El modelo de las partículas independientes.

Las funciones.

Las tendencias.

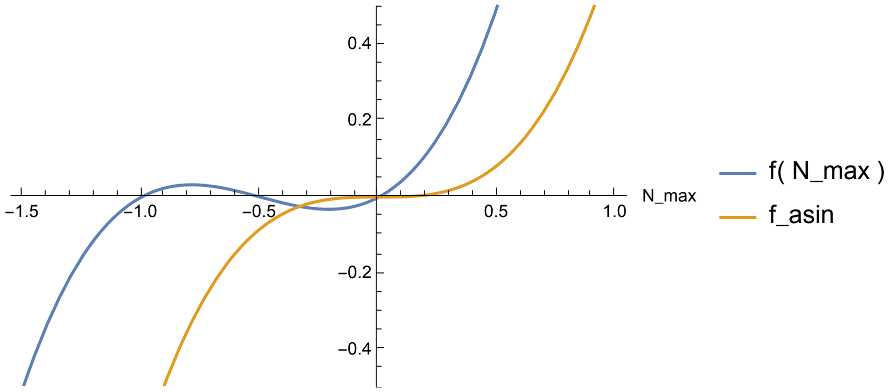
In[∘]:=
```
Plot[{x * (x + 1) * (2 * x + 1) / 3, 2 * x * x * x / 3}, {x, 0, 5},
 AxesLabel → {"N_max"}, PlotLegends → {"f( N_max )", "f_asin"}]
```

Out[∘]=



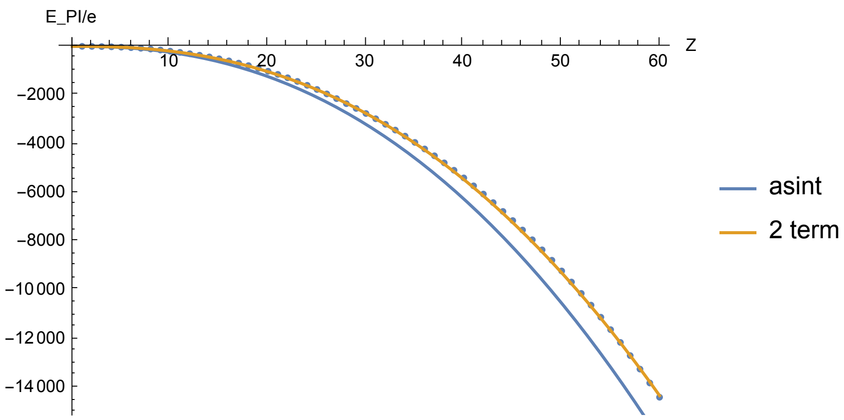
In[∘]:=
```
Plot[{x * (x + 1) * (2 * x + 1) / 3, 2 * x * x * x / 3},
 {x, -1.5, 1.0}, AxesLabel → {"N_max"},
 PlotLegends → {"f( N_max )", "f_asin"}, PlotRange → {-0.5, 0.5}]
```

Out[∘]=



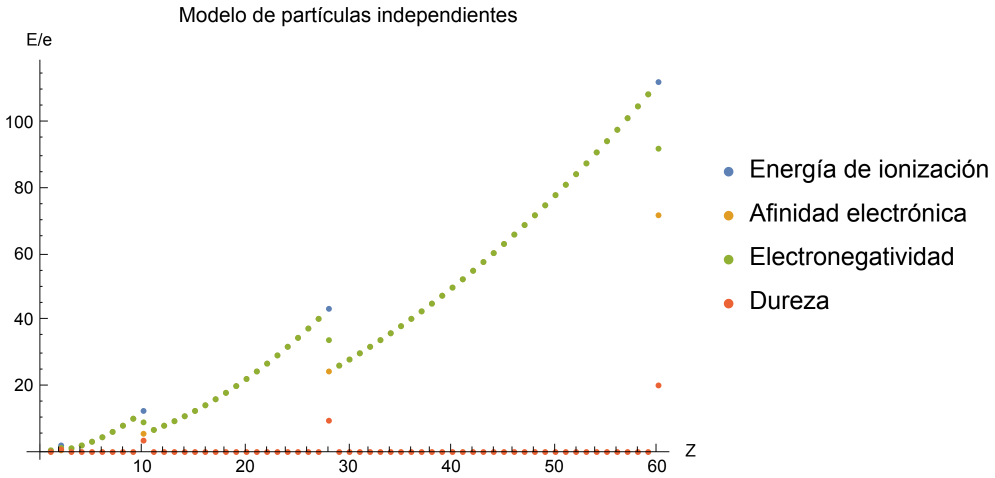
In[∘]:=
```
temp = Table[N[epi[n, n]], {n, 1, 60}];
Show[ListPlot[temp, AxesLabel → {"Z", "E_PI/e"}],
 Plot[{-x * x * (3 * x / 2) ^ (1 / 3), -x * x * ((3 * x / 2) ^ (1 / 3) - 1 / 2)},
  {x, 0, 60}, PlotLegends → {"asint", "2 term"}]]
```

Out[∘]=



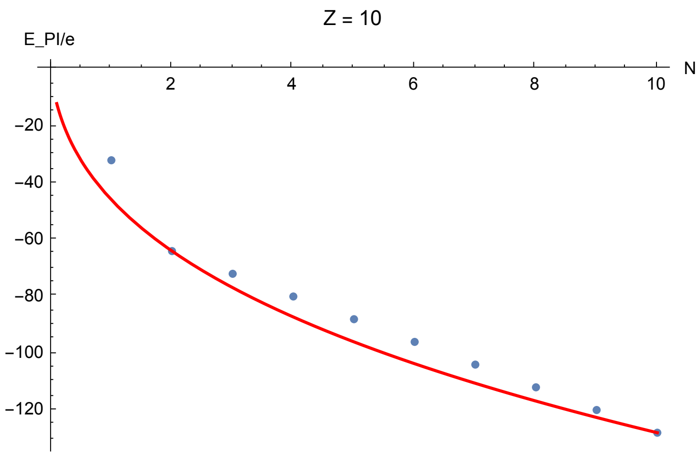
In[∘]:=
```
temp = {Table[N[epi[n - 1, n] - epi[n, n]], {n, 1, 60}],
    Table[N[epi[n, n] - epi[n + 1, n]], {n, 1, 60}],
    Table[N[-epi[n + 1, n] + epi[n - 1, n]] / 2, {n, 1, 60}],
    Table[N[epi[n + 1, n] - 2 * epi[n, n] + epi[n - 1, n]] / 2, {n, 1, 60}]};
ListPlot[temp, AxesLabel → {"Z", "E/e"},
 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[∘]=



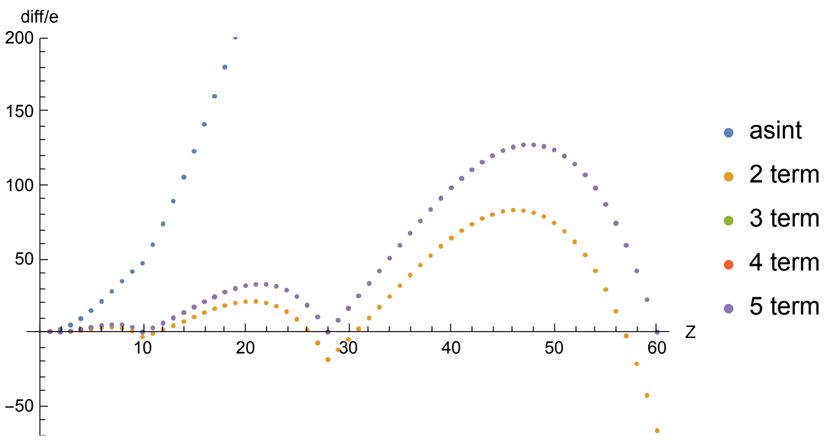
El análisis del modelo polinomial.

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

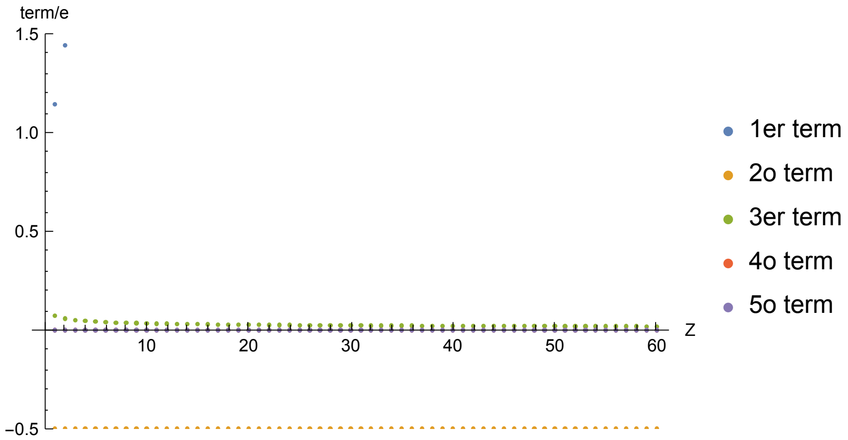
In[∘]:=
```
temp = {Table[epi[n, n] + n * n * (3 * n / 2) ^ (1 / 3), {n, 1, 60}],
   Table[epi[n, n] + n * n * ((3 * n / 2) ^ (1 / 3) - 1 / 2), {n, 1, 60}], Table[epi[n, n] +
     n * n * ((3 * n / 2) ^ (1 / 3) - 1 / 2 + 1 / 12 * (2 / (3 * n)) ^ (1 / 3)), {n, 1, 60}],
   Table[epi[n, n] + n * n * ((3 * 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}
```
Out[∘]= $\left\{\frac{77\,Z}{512}, \frac{77\,Z}{512}, 1\right\}$

1s 3s

In[∘]:=
```
{jhs = Js[n3s, n1s], khs = Ks[n3s, n1s], khs / jhs}
```
Out[∘]= $\left\{\frac{815\,Z}{8192}, \frac{189\,Z}{32\,768}, \frac{189}{3260}\right\}$

2s 3s

In[∘]:=
```
{jhs = Js[n3s, n2s], khs = Ks[n3s, n2s], khs / jhs}
```
Out[∘]= $\left\{\frac{32\,857\,Z}{390\,625}, \frac{73\,008\,Z}{9\,765\,625}, \frac{73\,008}{821\,425}\right\}$

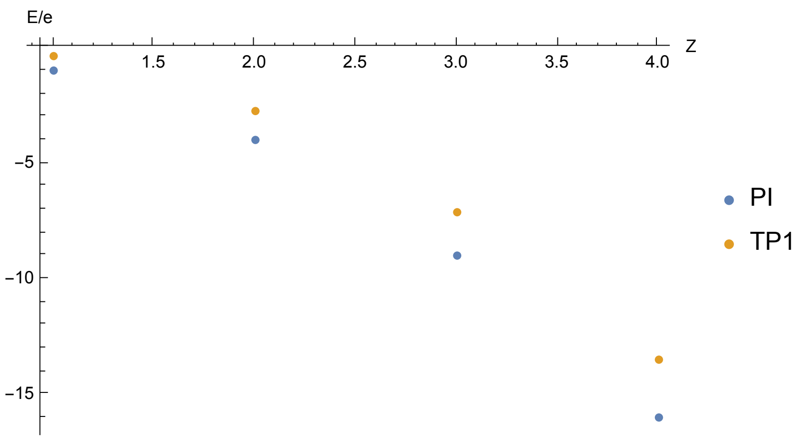
3s 3s

In[∘]:=
```
{jhs = Js[n3s, n3s], khs = Ks[n3s, n3s], khs / jhs}
```
Out[∘]= $\left\{\frac{17\,Z}{256}, \frac{17\,Z}{256}, 1\right\}$

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

Las funciones.

N = 2

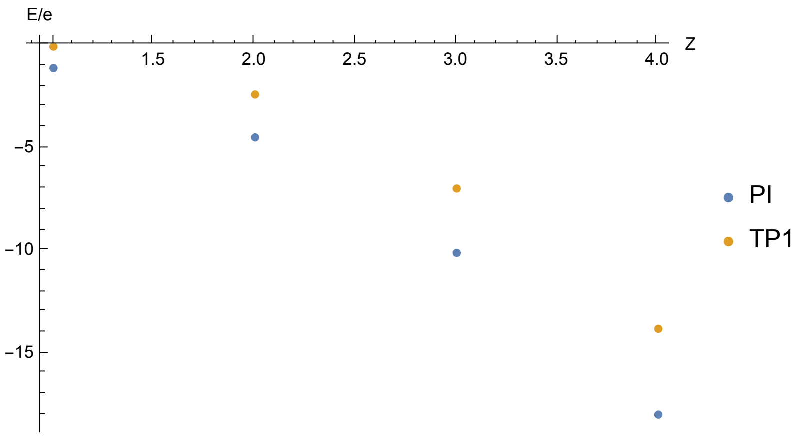
In[∘]:=
```
tempj1 = Js[n1s, n1s];
```
In[∘]:=
```
temp = {Table[{z, 2 * ehid[1, z]}, {z, 1, 4}],
    Table[{z, 2 * ehid[1, z] + tempj1 /. Z → z}, {z, 1, 4}]};
ListPlot[temp, AxesLabel → {"Z", "E/e"}, PlotLegends → {"PI", "TP1"}]
```
Out[∘]= 

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[•]=

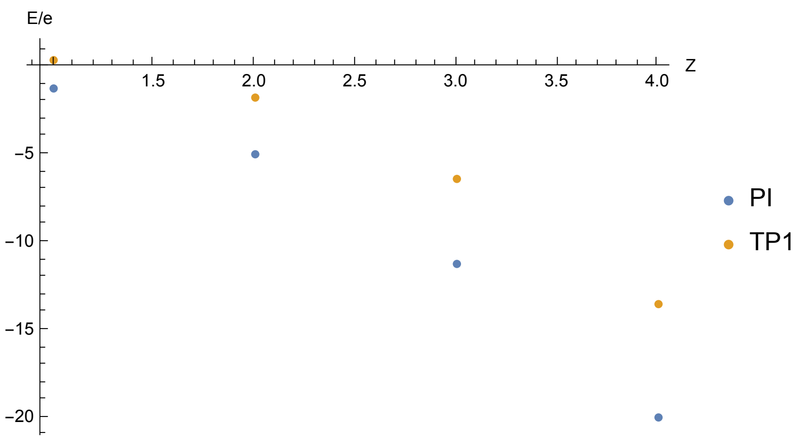


N = 4

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[•]=

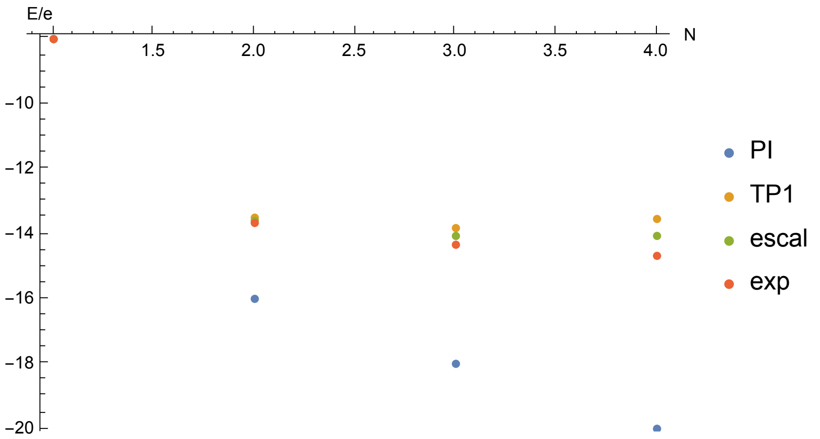


Z = 4

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.

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

4. La estructura molecular.