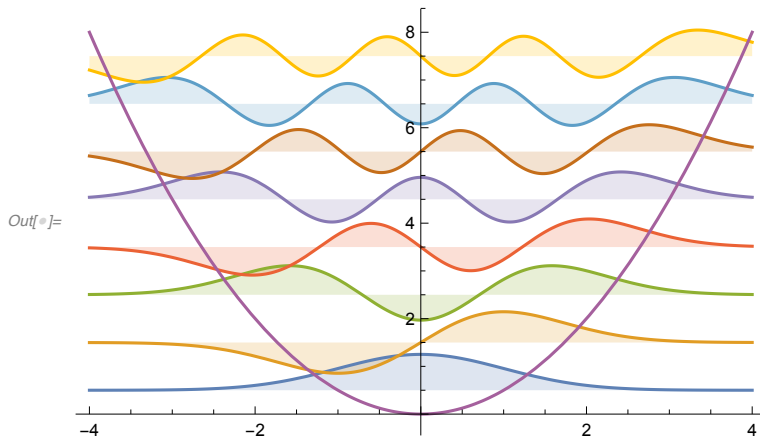```
In[ ]:= SetDirectory[NotebookDirectory[]];
        Import["init.wl"];
```

## Harmonic Oscillator

```
In[ ]:= f[n_, x_] := ((1 / Pi) ^ (1 / 4) HermiteH[n, x]) / (E ^ (x^2 / 2) Sqrt[2^n n!])
        Plot[Evaluate@
         Append[Table[f[n, x] + n + 1 / 2, {n, 0, 7}], x^2 / 2],
         {x, -4, 4}, Filling -> Table[n -> n - 1 / 2, {n, 1, 8}]]
```

Out[ ]=

Particle in finite well

```
In[ ]:= subs = {ρ → Sqrt[-2 m en] / ℏ, k → Sqrt[2 m (en + Vo)] };
        ϕ1[x_] := l1 Exp[ρ x] ;
        ϕ2s[x_] := w1 Cos[k x];
        ϕ2a[x_] := w1 Sin[k x];
        ϕ3[x_] :=  r2 Exp[-ρ x];
```

```
In[ ]:= sym = {ϕ1[-a] - ϕ2s[-a] == 0, (D[ϕ1[x], x] - D[ϕ2s[x], x] == 0) /. x → -a}
Out[ ]= {e^(-a ρ) l1 - w1 Cos[a k] == 0, e^(-a ρ) l1 ρ - k w1 Sin[a k] == 0}
```

```
In[ ]:= asym = {ϕ1[-a] - ϕ2a[-a] == 0, (D[ϕ1[x], x] - D[ϕ2a[x], x] == 0) /. x → -a}
Out[ ]= {e^(-a ρ) l1 + w1 Sin[a k] == 0, e^(-a ρ) l1 ρ - k w1 Cos[a k] == 0}
```

```
In[ ]:= subs = {ρ → Sqrt[-2 m en] / ℏ, k → Sqrt[2 m (en + Vo)] };


        f1[en_] := Sqrt[ -en / (en + Vo) ] ;

        fs[en_] := Tan[a Sqrt[2 m (en + Vo)] / ℏ ] /. subs;
        fa[en_] := -Cot[a Sqrt[2 m (en + Vo)] / ℏ] /. subs;
        params = {a → 2, m → 1, ℏ → 1, Vo → 10};


        rs0 = FindRoot[(f1[en] - fs[en] == 0) /. params, {en, -9.999}] // Chop;
        rs1 = FindRoot[(f1[en] - fs[en] == 0) /. params, {en, -8}] // Chop;
        rs2 = FindRoot[(f1[en] - fs[en] == 0) /. params, {en, -4}] // Chop;
```

```
ra1 = FindRoot[(f1[en] - fa[en] == 0) /. params, {en, -9}] // Chop;
ra2 = FindRoot[(f1[en] - fa[en] == 0) /. params, {en, -6}] // Chop;
ra3 = FindRoot[(f1[en] - fa[en] == 0) /. params, {en, -2}] // Chop;


tab1 = {{en /. rs0, S}, {en /. rs1, S},
    {en /. rs2, S}, {en /. ra1, A}, {en /. ra2, A}, {en /. ra3, A}};
tab1 // TableForm

p1 = {en /. rs0, f1[en /. rs0] /. params};
p2 = {en /. rs1, f1[en /. rs1] /. params};
p3 = {en /. rs2, f1[en /. rs2] /. params};
p4 = {en /. ra1, f1[en /. ra1] /. params};
p5 = {en /. ra2, f1[en /. ra2] /. params};
p6 = {en /. ra3, f1[en /. ra3] /. params};

Plot[{f1[x] /. params,
   fs[x] /. params,
   fa[x] /. params
 }, {x, -10, 0},
 PlotRange → {0, 10},
 PlotStyle → {{Thick, Dashing[{0.01}]}, Thick, Thick},
 AxesLabel → {"E", None},
 LabelStyle → 16,
 AspectRatio → 1,
 Exclusions → {Sin[2 √(2 (x + 10))] == 0, Cos[2 √(2 (x + 10))] == 0},
 PlotPoints → 75,
 Epilog → {
   Disk[{en /. rs0, f1[en /. rs0] /. params}, 0.1],
   Disk[{en /. rs1, f1[en /. rs1] /. params}, 0.1],
   Disk[{en /. rs2, f1[en /. rs2] /. params}, 0.1],
   Disk[{en /. ra1, f1[en /. ra1] /. params}, 0.1],
   Disk[{en /. ra2, f1[en /. ra2] /. params}, 0.1],
   Disk[{en /. ra3, f1[en /. ra3] /. params}, 0.1],
   Style[Text["S", p1 + {0.4, 0}], 18],
   Style[Text["S", p2 + {0.4, 0}], 18],
   Style[Text["S", p3 + {0, 0.4}], 18],
   Style[Text["A", p4 + {0.4, 0}], 18],
   Style[Text["A", p5 + {0, 0.4}], 18],
   Style[Text["A", p6 + {0, 0.4}], 18],
   AxesStyle → Thick
  }]
```
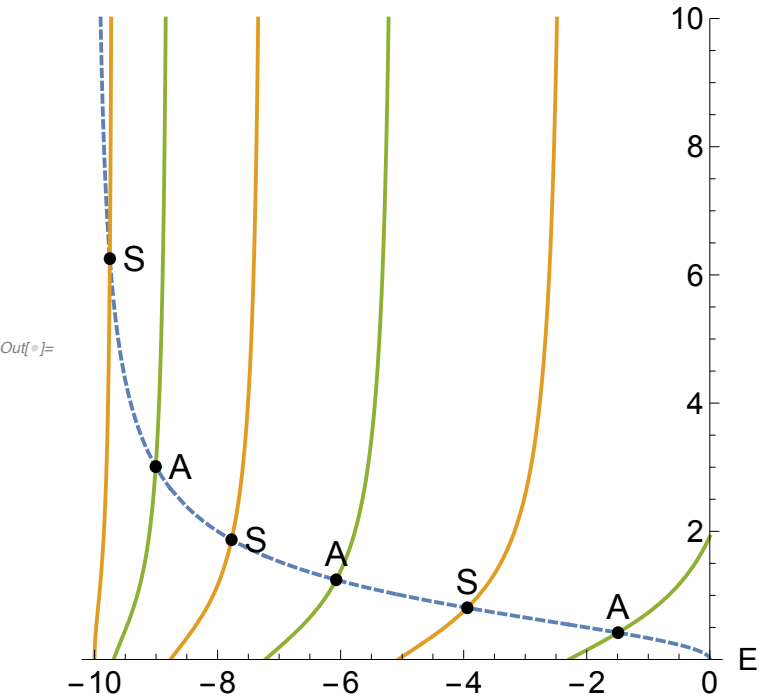
Out[ ]//TableForm=
```
−9.7507      S
−7.77297     S
−3.94146     S
−9.00542     A
−6.07186     A
−1.49125     A
```
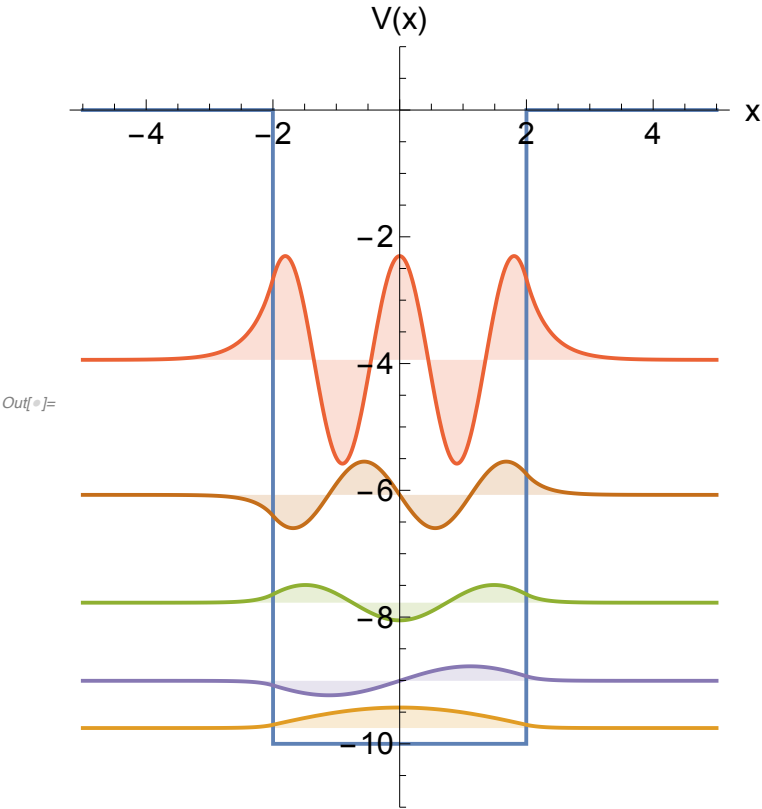
Out[ ]=

```mathematica
In[◦]:= subs = {ρ → √(-2 m en) / ℏ, k → √(2 m (en + Vo)) } /. params;
     ψs[x_] := Which[
             Abs[x] < a, B Cos[ √(2 m (en + Vo)) x],
             x ≥ a,  Exp[-x √(-2 m en) ],
             x ≤ -a, Exp[ x √(-2 m en) ]] /. {B → Sec[a √(2 m (en + Vo)) ] Exp[-a √(-2 m en) ]}
     ψa[x_] := Which[
             Abs[x] ≤  a, B Sin[ √(2 m (en + Vo)) x] /. subs,
             x > a,  Exp[-x √(-2 m en) ],
             x < -a, -Exp[ x √(-2 m en) ]] /.
       {B → Csc[a √(2 m (en + Vo)) / ℏ] Exp[-a √(-2 m en) / ℏ ]}
     V[x_] := If[Abs[x] < a, -Vo, 0];

     amp = 350;
     plotWF = Plot[{
         V[x] /. params,
         (amp ψs[x] + en) /. Join[params, rs0],
         (amp ψs[x] + en) /. Join[params, rs1],
         (amp ψs[x] + en) /. Join[params, rs2],
         ( amp ψa[x] + en) /. Join[params, ra1],
         ( amp ψa[x] + en) /. Join[params, ra2]
       }, {x, -5, 5},
       Filling → {
         2 -> en /. Join[params, rs0],
         3 -> en /. Join[params, rs1],
         4 -> en /. Join[params, rs2],
         5 -> en /. Join[params, ra1],
         6 -> en /. Join[params, ra2],
        },
       PlotRange → {1, -11},
       LabelStyle → 16,
       AspectRatio → {1},
       PlotStyle → Thick,
       AxesLabel → {"x", "V(x)"}];
     Show[plotWF]
```

DOS versus dimensionality

```
In[•]:= ρ[d_, x_] := 2^(d/2-1) d π^(d/2-2) (√(m x) / ℏ)^d / (x Gamma[(d / 2 + 1)])

    Plot[
     {ρ[1, x] /. {m → 1, ℏ → 1},
      ρ[2, x] /. {m → 1, ℏ → 1},
      ρ[3, x] /. {m → 1, ℏ → 1},
      ρ[4, x] /. {m → 1, ℏ → 1},
      ρ[5, x] /. {m → 1, ℏ → 1}
     }, {x, 0, 1},
     PlotStyle → Thick,
     AspectRatio → 1,
     AxesLabel → {"E (a.u)", "ρ_d(E)"},
     LabelStyle → 16,
     Epilog → {
       Style[Text["1D", {0.8, 0.3}], 16],
       Style[Text["2D", {0.8, 0.8}], 16],
       Style[Text["3D", {0.8, 1.75}], 16],
       Style[Text["4D", {0.8, 3.4}], 16],
       Style[Text["5D", {0.8, 6.0}], 16]
      }]
```

Out[•]=