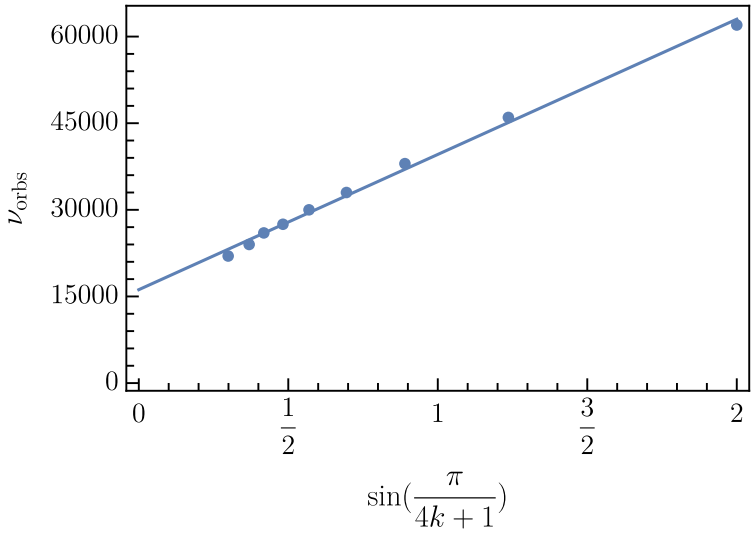
```
SetDirectory[NotebookDirectory[]];
Import["init.wl"];
```

Variation of Slater Orbital Overlap

```
orbs = {{1, 62 000}, {2, 46 000}, {3, 38 000}, {4, 33 000},
   {5, 30 000}, {6, 27 500}, {7, 26 000}, {8, 24 000}, {10, 22 000}};
free[k_] := 1.54 10^5/(2 k + 1);
huck[k_] := 4 β Sin[π/(4 k + 2)];
```

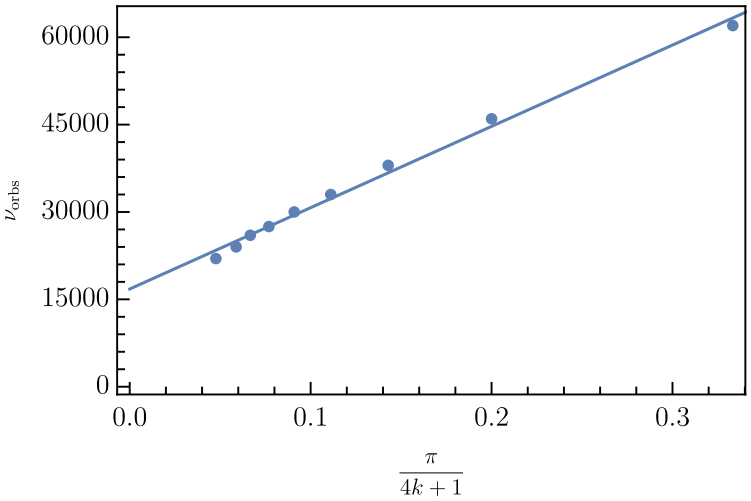
```
kval = {1, 2, 3, 4, 5, 6, 7, 8, 10};
huck[kval] / (4 β) ;
nuOrbs = Transpose[orbs][[2]];
d1 = Transpose[{huck[kval] / (β), nuOrbs}];
d2 = Transpose[{free[kval] / (1.54 * 10^5), nuOrbs}];
p1a = ListPlot[
   d1,
   PlotMarkers → Automatic,
   Joined → False];
p2a = ListPlot[
   d2,
   PlotMarkers → Automatic,
   Joined → False];

f1 = Fit[d1, {1, x}, x];
a1 = f1 /. x → 0;
b1 = D[f1, x];
huckfit = Transpose[{kval, a1 + huck[kval] /. β → b1}];
f2 = Fit[d2, {1, x}, x];
a2 = f2 /. x → 0;
b2 = D[f2, x];

p1b = Plot[f1, {x, 0, 2}];
p2b = Plot[f2, {x, 0, 1.5}];
Show[p1a, p1b, FrameLabel →
  {tex["\\sin(\\frac{\\pi}{4k+1})", 16], tex["\\nu_\\text{orbs}", 16]},
 FrameTicks → {{tf[0, 60 000, 4, 5, 10.5 * 100 / 72, 10], None},
   {tf[0, 2, 4, 5, 10.5 * 100 / 72, 10], None}},
 Frame → True,
 ImageSize → 10 * 100 / 2.54,
 FrameStyle → Directive[Black, AbsoluteThickness[1]]
]
linfit = Transpose[{kval, b2/(2 kval + 1) + a2}];
```

Out[•]=



In[•]:=
```
Show[p2a, p2b,
 FrameLabel → {MaTeX["\\frac{\\pi}{4k+1}"], MaTeX["\\nu_\\text{orbs}"]},
 FrameTicks → {{tf[0, 60 000, 4, 5, 10.5 * 100 / 72, 10], None},
   {tf[0, 0.4, 4, 5, 10.5 * 100 / 72, 10], None}},
 Frame → True,
 ImageSize → 10 * 100 / 2.54,
 FrameStyle → Directive[Black, AbsoluteThickness[1]]
]
```

Out[•]=



In[•]:=
```
data = Transpose[ {kval, free[kval], a1 + huck[kval] /. β → b1 , nuOrbs}];
TableForm[data]
```

Out[•]//TableForm=

1	51 333.3	63 009.7	62 000
2	30 800.	45 119.1	46 000
3	22 000.	37 016.5	38 000
4	17 111.1	32 438.3	33 000
5	14 000.	29 503.1	30 000
6	11 846.2	27 463.	27 500
7	10 266.7	25 963.4	26 000
8	9058.82	24 814.9	24 000
10	7333.33	23 172.	22 000

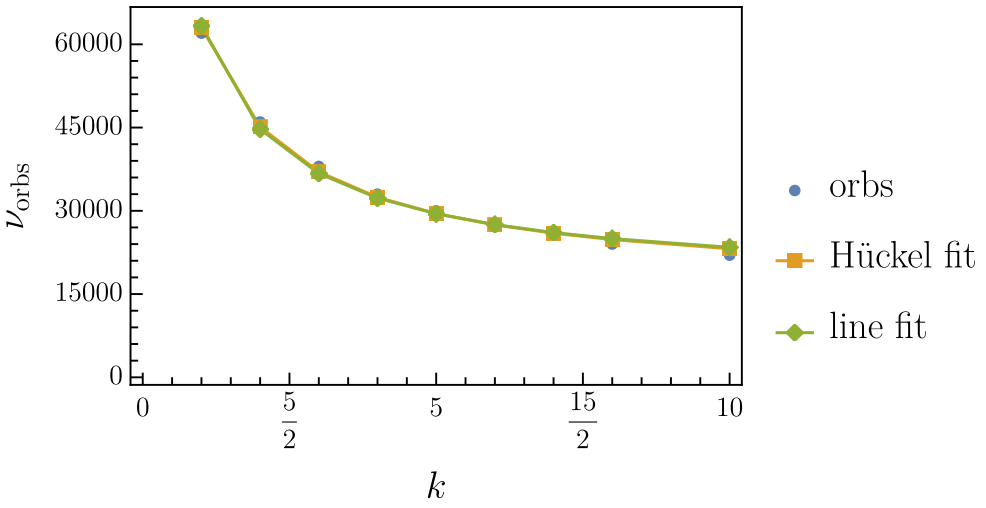
In[•]:=
```
TableForm[orbs]
```

Out[•]//TableForm=

1	62 000
2	46 000
3	38 000
4	33 000
5	30 000
6	27 500
7	26 000
8	24 000
10	22 000

In[•]:=
```
p1 = ListPlot[{orbs, huckfit, linfit}, Joined → {False, True, True},
  PlotMarkers → {Automatic}, PlotLegends → {tex["\\text{orbs}", 20],
    tex["\\text{H\\\"uckel fit}", 20], tex["\\text{line fit}", 20]},
  FrameLabel → {tex["k", 20], tex["\\nu_\\text{orbs}", 20]},
  FrameTicks → {{tf[0, 60 000, 4, 5, 10.5 * 100 / 72, 10], None},
    {tf[0, 10, 4, 5, 10.5 * 100 / 72, 10], None}},
  Frame → True,
  ImageSize → 10 * 100 / 2.54,
  FrameStyle → Directive[Black, AbsoluteThickness[1]]]
```

Out[•]=



In[•]:=
```
slaterOrb[r_] := Exp[-p] (1 + p + 2 p^2 / 5 + p^3 / 15) /. {p → 1.626 r / 0.52}
guess = Series[slaterOrb[r], {r, 1.39, 1}] // Normal
```

Out[•]=
```
0.238038 - 0.409956 (-1.39 + r)
```

In[•]:=
```
p1 = Plot[slaterOrb[r], {r, 0, 3},
    AspectRatio → 1,
    AxesLabel → {tex["R(\\text{A})", 20], tex["S(2p\\pi,2p\\pi)", 20]},
    Ticks →
     {tf[0, 3.0, 4, 5, 10.5 * 100 / 72, 10], tf[0, 1.0, 4, 5, 10.5 * 100 / 72, 10]},
    LabelStyle → 16];
p2 = Plot[guess, {r, 1.1, 1.6}, PlotStyle → Thick];
Show[p1, p2,
 Epilog → {Line[{{1.39, slaterOrb[1.39]}, {1.39, 0}}]}]
```

Out[•]=