Physics 601, Homework I

Problemw 1 and 2; To solve these problems I simply used Eq. (15) of the notes and computed B(E) using that $\phi_{\rm in}(r) = A\sqrt{2(E+V_0)}$ for both positive and negative E. Then $B(E) = k_{in}(E)\cot[k_{\rm in}(E)r_0]$, where $k_{\rm in}(E) = \sqrt{2(E+V_0)}$. This is then substituted into Eq.(15) to get $K = \tan\delta(E)$. The attached Mathematica notebook shows a plot of the phase shift for $E > 0$. But we can also use the same formulas for $E < 0$ to find where $K = i$. Plots are also shown where the one bound state is located. A check is made to see that there is no bound state close to $E = 0$. Finally, since $\ell = 0$ solutions are simply sin functions the solution was also obtained by matching the functions directly using $\phi(r) = A\sin(k_{\rm in}r + \delta)$ and $\phi_{\rm in} = A_{\in}\sin(kr)$ as a check. Notice that when using the arctan function it is necessary to eliminate jumps by π in the phase shift to obtain a smooth plot.

Problem 3. In this case it is easier match solutions at boundaries directly. There are three regions call them $j = 0, 1, 2$. In each region the solution is $\phi_j = A_j\sin(k_j r + \delta_j])$. The functions and their derivatives are matched at the boundaries $r_j,\ j = 0, 1$ using that $\delta_0 = 0$. This gives the equations

$$k_{j+1}\cot(k_{j+1}r_j + \delta_j) = k_j\cot(k_j r_j + \delta_j), \quad j = 0, 1 \tag{1}$$

so that

$$\delta_2 \ = \ \delta = \text{arccot}((k_1/k_2)\cot(k_1 r_1 + \delta_1)) - k_2 r_1 \tag{2}$$

$$\delta_1 \ = \ \text{arccot}((k_0/k_1)\cot(k_0 r_0 + \delta_0)) - k_1 r_0 \tag{3}$$

$$\delta_0 \ = \ 0 \tag{4}$$

These equations can be used for all E, provide one takes $\sqrt{-C} = i\sqrt{C}, C > 0$. Mathematica does this automatically. The second attached notebook shows the solution in this case. Note that there are lot of jumps by π.

We could also use equation (15) or (16) of the notes. In this case $B(E) = k_1\cot(k_1 r_1 + \delta_1)$ is the logarithmic derivative at the boundary to the outer region.

Use of B(E) matrix for a square well

■ Set up u, v, uin, derivatives, and B(E) (mainly inner region)

```
V0 = 2.
```

```
2.
```

```
u[x_] := Sin[x]
```

```
v[x_] := Cos[x]
```

```
kin[V0_, en_] := Sqrt[2 * (en + V0)]
```

```
B[en_, r_] := kin[V0, en] * Cot[kin[V0, en] * r]
```

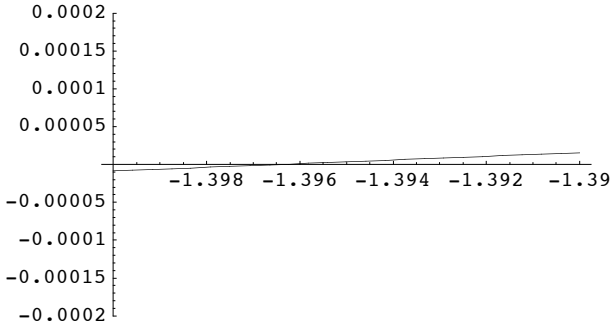
■ Set up K=Tan(delta) (mainly outer region).

```
k[en_] := Sqrt[2 * en]
```

```
K[en_, r0_] :=
 -u[k[en] * r0] / v[k[en] * r0] + (k[en] / v[k[en] * r0] ^ 2) / (B[en, r0] + k[en] * Tan[k[en] * r0])
```

■ Find values of energy for which K=-i.

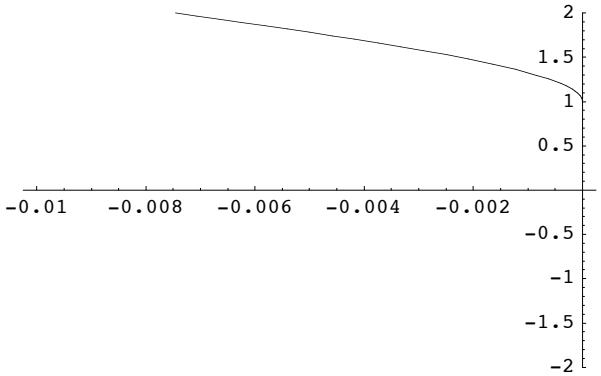
```
Plot[Im[K[en, 2.33] + I], {en, -1.4, -1.39}, PlotRange → {-.0002, .0002}];
```




```
K[-1.398, 2.333]
```

```
0. - 1. i
```

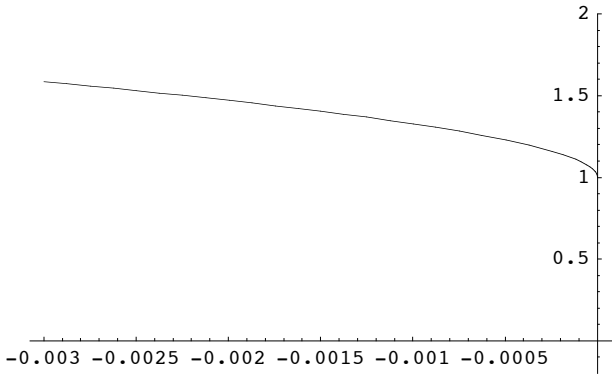
```
Plot[Im[K[en, 2.33] + I], {en, -.01, -0}, PlotRange → {-2, 2}];
```




```
K[-0.000001, 2.33]
```

```
0. + 0.0101899 i
```

```
Plot[Im[K[en, 2.33] + I], {en, -.003, -.0}, PlotRange → {-.2, 2}];
```




```
K[-0.000001, 2.33] / k[-0.000001]
```

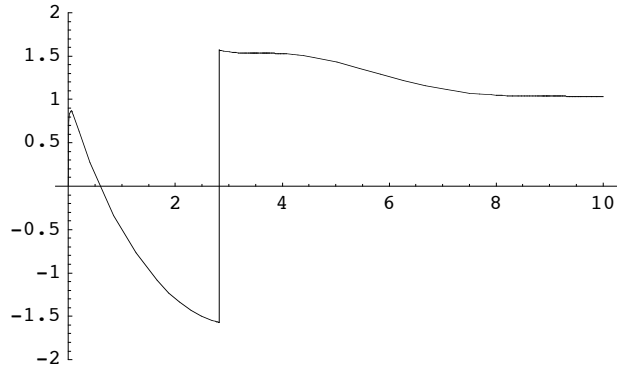
```
7.20538 + 0. i
```

We see that there is one bound state, at about E=-1.4. There is no bound state at k=0.0

■ Find the phase shift delta(E).

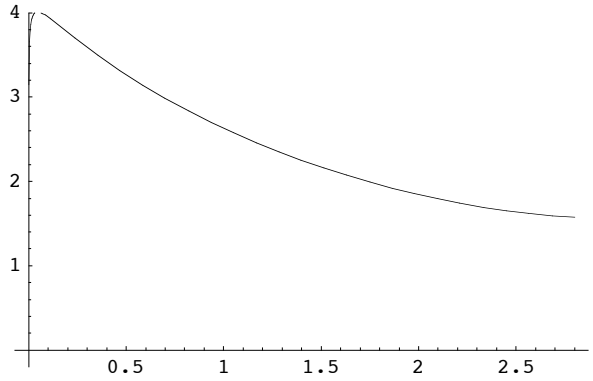
```
delta[en_, r0_] := ArcTan[K[en, r0]]
```

```
Plot[delta[en, 2.33], {en, 0, 10.}, PlotRange → {-2, 2}];
```

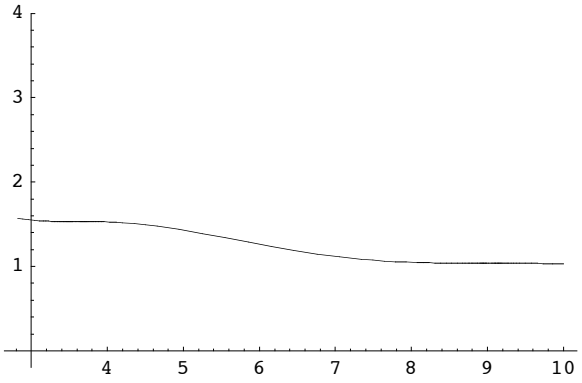


Eliminate the break at E~3 au. The steps to do this are given below.

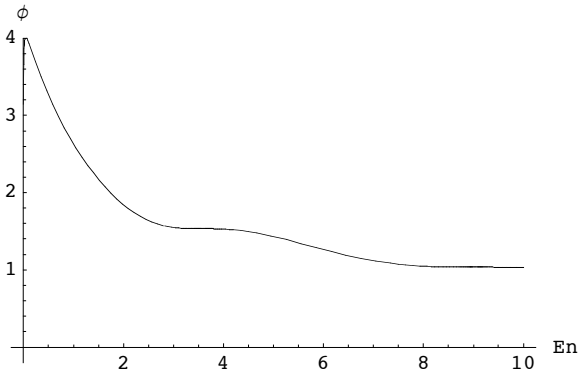
```
p1 = Plot[delta[en, 2.33] + Pi, {en, 0, 2.8}, PlotRange → {-0.2, 4}];
```




```
p2 = Plot[delta[en, 2.33], {en, 2.82, 10}, PlotRange → {-.2, 4}];
```



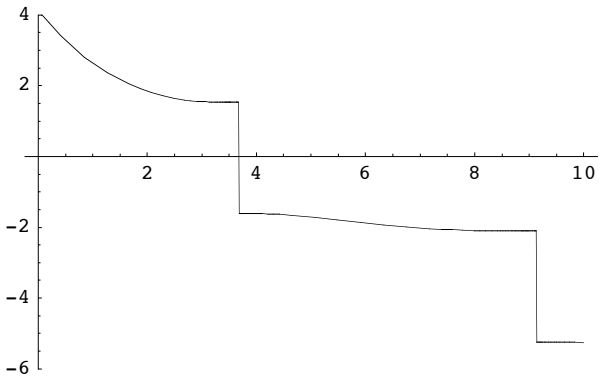
```
pf = Show[p1, p2, AxesLabel → {En, ϕ}];
```



The breaks have now been completely eliminated.

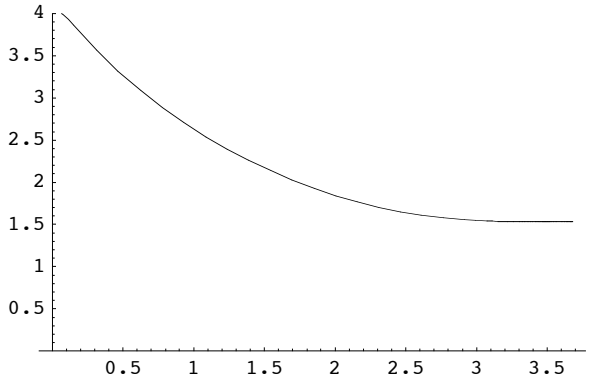
■ Check: Use a more direct solution.

```
deltaa[en_, r0_] := ArcTan[(k[en] / kin[V0, en]) * Tan[kin[V0, en] * r0]] - k[en] * r0

p1a = Plot[deltaa[en, 2.33] + 2 * Pi, {en, 0.001, 10}, PlotRange → {-6, 4}];
```

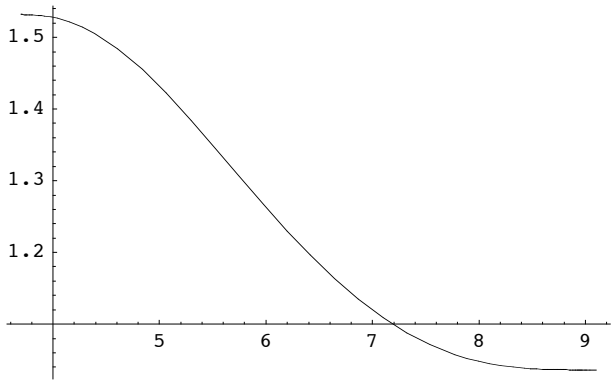


Eliminate the breaks. Note that this way shows 3 breaks.

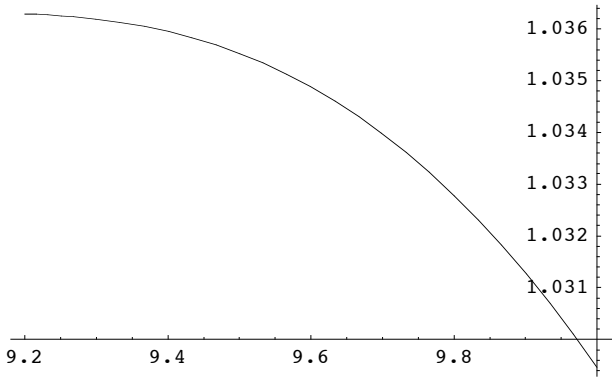
```
p1a = Plot[deltaa[en, 2.33] + 2 * Pi, {en, 0.001, 3.68}, PlotRange → {0, 4}];
```



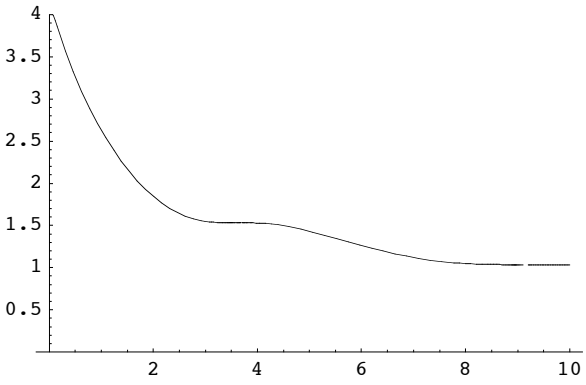
```
p2a = Plot[deltaa[en, 2.33] + 3 * Pi, {en, 3.7, 9.1}];
```



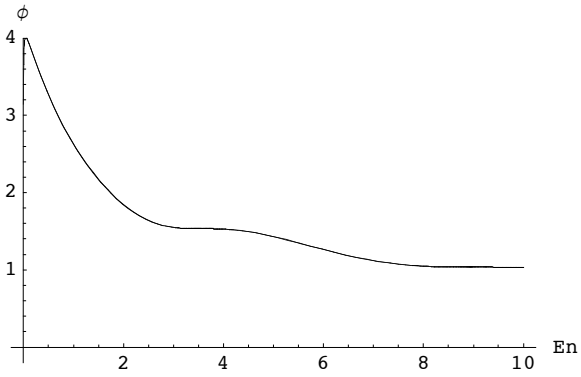

```
p3a = Plot[deltaa[en, 2.33] + 4 * Pi, {en, 9.2, 10}];
```




```
pfp = Show[p1a, p2a, p3a];
```

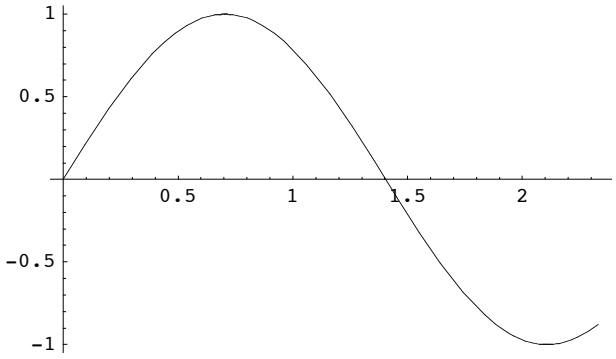


```
Show[pf, pfp];
```

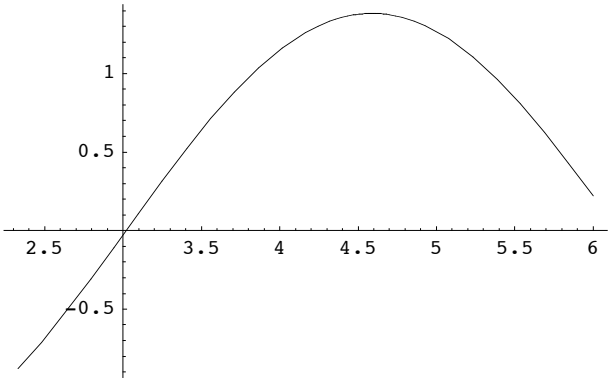


This plot shows that the same phase shift is obtained both ways.

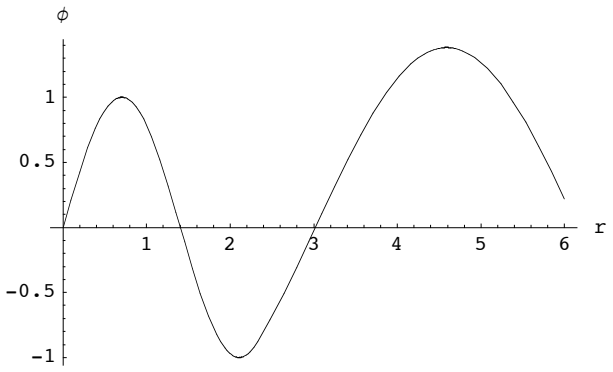
```
Phiin[en_, r_] := Sin[kin[2, en] * r]
delt[en_, r0_] := ArcTan[K[en, r0]]
Phi[en_, r_, r0_] :=
 Sin[k[en] * r + delt[en, r0]] * (Sin[kin[2, en] * r0] / Sin[k[en] * r0 + delt[en, r0]])

Phiin[en_, r_] := Sin[kin[2, en] * r]

p1 = Plot[Phiin[.5, r], {r, 0, 2.33}];
```




```
p2 = Plot[Phi[.5, r, 2.33], {r, 2.33, 6}];
```



```
Show[p1, p2, AxesLabel → {r, ϕ}]
```

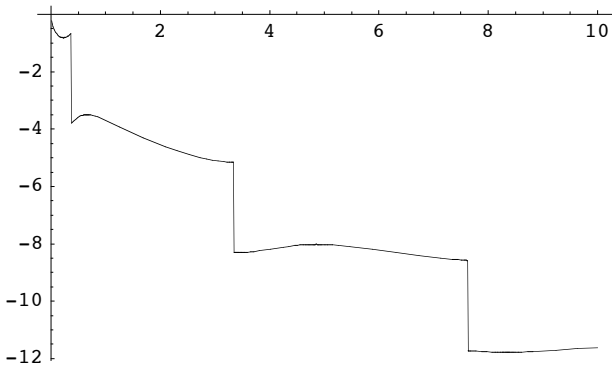



```
- Graphics -
```

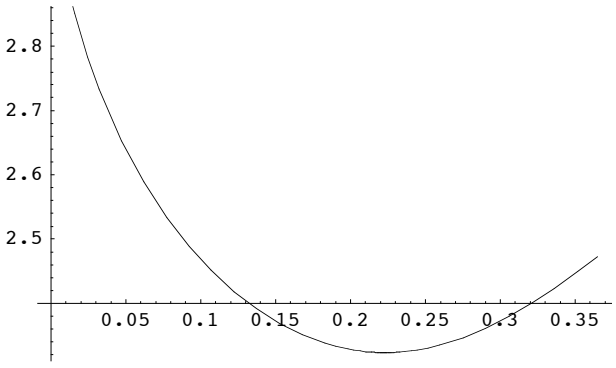
Above is a plot of the wave function ϕ vs. r for E=0.5 au.

■ Program for Eqs. (2) and (3) of the answer sheet

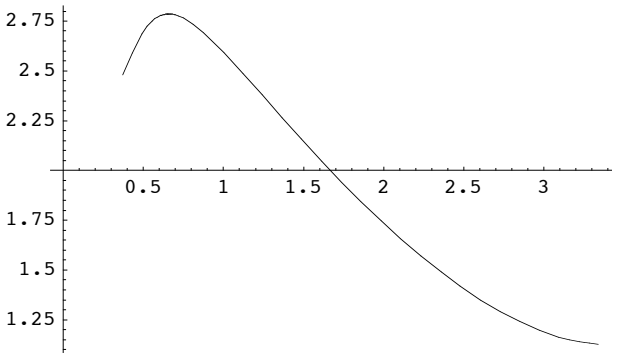
```
k0[en_] := Sqrt[2 * (en + 2.)]

k1[en_] := Sqrt[2 * (en - 2.)]

k2[en_] := Sqrt[2 * (en)]

r0 = 2.33

2.33

r1 = 2.6

2.6

Clear[delta1]

delta1[en_] := ArcCot[(k0[en] / k1[en]) * Cot[k0[en] * r0]] - k1[en] * r0

delta2[en_] := ArcCot[(k1[en] / k2[en]) * Cot[k1[en] * r1 + delta1[en]]] - k2[en] * r1

Plot[delta2[en], {en, 0.01, 10}];
```



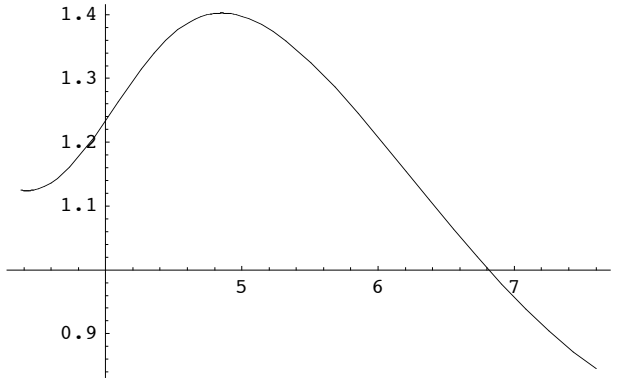

```
p1 = Plot[delta2[en] + Pi, {en, 00.001, 0.365}];
```



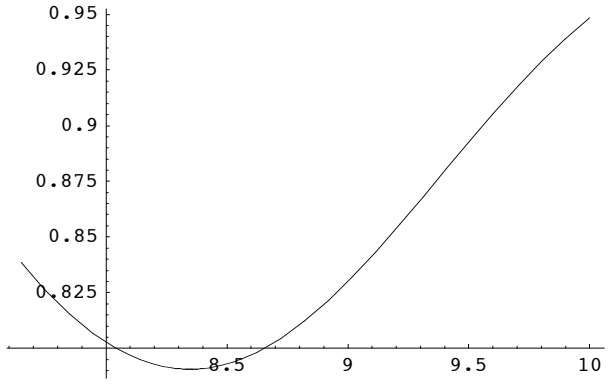
```
p2 = Plot[delta2[en] + 2 * Pi, {en, 0.37, 3.34}];
```



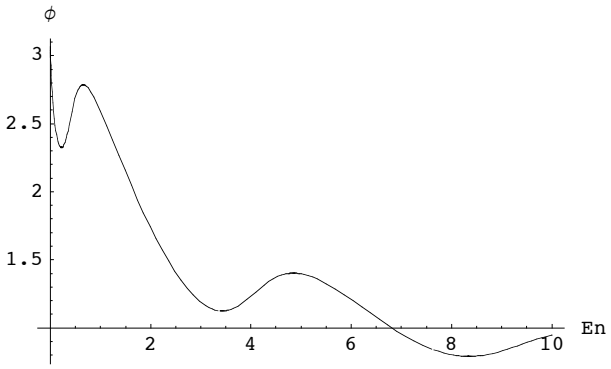

```
p3 = Plot[delta2[en] + 3 * Pi, {en, 3.38, 7.6}];
```



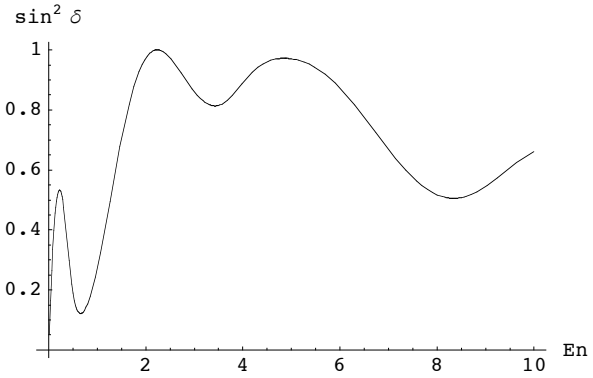

```
p4 = Plot[delta2[en] + 4 * Pi, {en, 7.65, 10}];
```



```
Show[p1, p2, p3, p4, AxesLabel → {En, ϕ}];
```



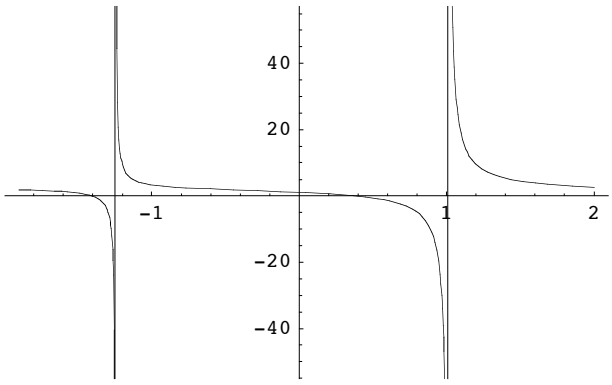

```
Plot[Sin[delta2[en]]^2, {en, 0.01, 10}, AxesLabel -> {En, sin^2 (δ)} ];
```



We have not discussed this yet, but the sin^2 of the phase shift is the physically significant paramter. It is a smooth function of the phase shift and does not show the effects of jumps.

We can also calculate B(E) from the logarithmic derivative of the inner function at r=r1.

```
B[en_] := k1[en] * Cot[k1[en] * r1 + delta1[en]]

Plot[B[en], {en, -1.9, 2}];
```



Notice that B(E) is real for all values of E. It is an analytic function of E except at the first order poles where it becomes infinite.

Use of B(E) matrix for a square well

■ Set up u, v, uin, derivatives, and B(E) (mainly inner region)

```
V0 = 2
```

```
2
```

```
u[x_] := Sin[x]
```

```
v[x_] := Cos[x]
```

```
kin[V0_, en_] := Sqrt[2 * (en + V0)]
```

```
B[en_, r_] := kin[V0, en] * Cot[kin[V0, en] * r]
```

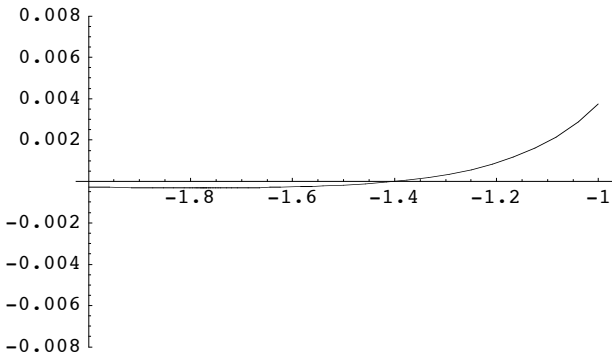
■ Set up K=Tan(delta) (mainly outer region).

```
k[en_] := Sqrt[2 * en]
```

```
K[en_, r0_] :=
 -u[k[en] * r0] / v[k[en] * r0] + (k[en] / v[k[en] * r0] ^ 2) / (B[en, r0] + k[en] * Tan[k[en] * r0])
```

■ Find values of energy for which K=-i.

```
Plot[Im[K[en, 2.33] + I], {en, -2, -1}, PlotRange → {-.008, .008}];
```

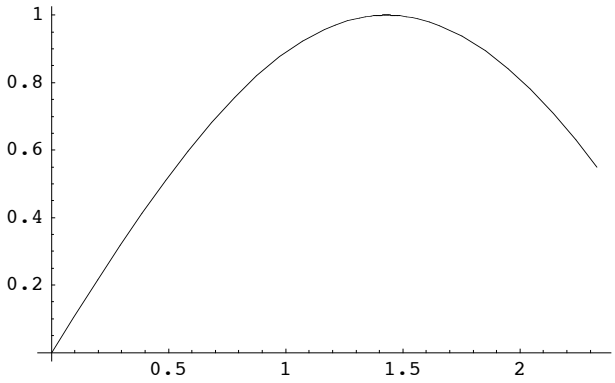



```
K[-1.396416, 2.33] + I
```

```
0. - 4.01306 × 10^-10 i
```

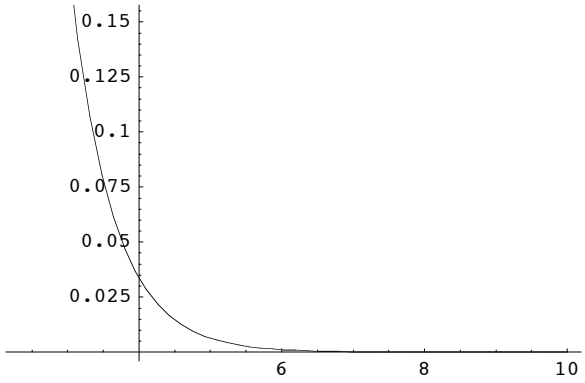
This verifies that the bound state energy is -1.396416 au ~ -1.4 au. The wave function is shown below.

```
p1 = Plot[Sin[kin[V0, -1.396416] * r], {r, 0, 2.33}];
```



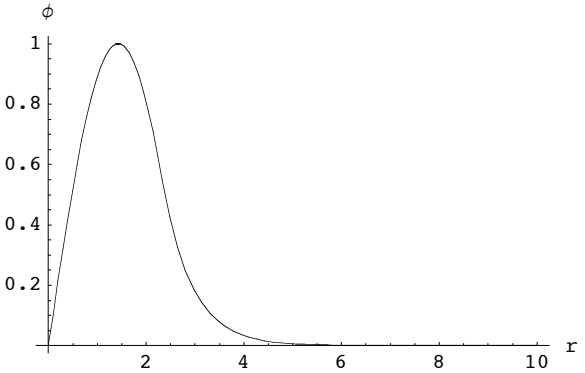

```
- Graphics -
```

```
p2 = Plot[Sin[kin[V0, -1.396416] * 2.33] * Exp[I * k[-1.396416] * (r - 2.33)], {r, 2.33, 10}];
```




```
- Graphics -
```

```
Show[p1, p2, AxesLabel → {r, ϕ}];
```



The above is a graph of the un-normalized wave function.