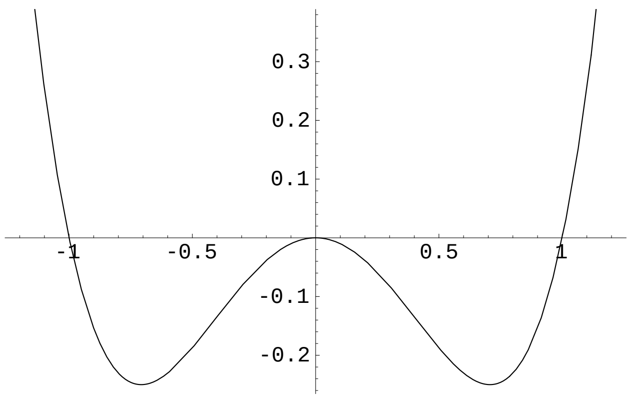
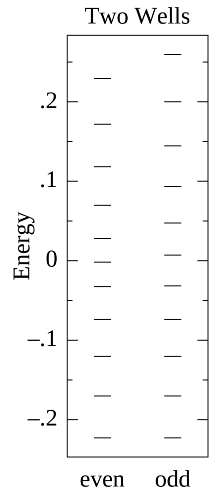
Consider the Quantum Mechanics of motion in a 1-d 'wine bottle bottom' potential $V(x) = x^2(x^2-1)$ as shown below with the corresponding stack of energy levels sorted by parity.





The Hamiltonian for this system

$$H = -\frac{\hbar^2}{2m}\,\partial_x^2 + x^2(x^2-1)$$

depends on a free parameter which we have chosen: $2m/\hbar^2 = 2628.8256429 \equiv \alpha^2$. (This results in the 20^{th} state having eigenenergy $E = .2$.) To appreciate the wave-functions of this Hamiltonian, page through the plots in the file `2well_all_psi.pdf`. Note now that for $E < 0$ the even/odd states are nearly degenerate, where as for $E > 0$ the even/odd states interleave as usual.

We aim to estimate the eigenenergies of this potential using the WKB approximation: plot the WKB integral as a function of E and pick out the spots where the result equals $\pi(n - \frac{1}{2})$.

An interesting feature of this potential is that the classical turning points differ significantly between case (A) with $E > 0$ and symmetrical turning points $\pm a$ and case (B) with $E < 0$ and asymmetrical turning points: either in the $x > 0$ well ($b < x < a$) or the $x < 0$ well ($-a < x < -b$) . Quantum mechanics tells us that because of tunneling a particle will not be located in just one well; instead it will end up equally distributed in both wells. The $E < 0$ states (in fact all states) will be either even or odd (the parity operator commutes with this symmetric potential) but $|\psi|^2$ will be the same in the two wells. Again, you should look through `2well_all_psi.pdf` to appreciate this result.

A distracting feature of this problem is that *Mathematica* balks at calculating the WKB integral. An old integral table by Gradshteyn & Ryzhik will provide needed answers.

Because the potential is a special quartic (a quadratic in x^2) its easy to find the turning points:

```
alpha=Sqrt[2628.8256429]
Solve[x^2(x^2-1)==e,x]
a = x /. Last[%]
b = x /. %%[[2]]
```

Note: b will be complex if $E > 0$.

The required WKB integral is:

$$\int \alpha\sqrt{E - x^2(x^2 - 1)}\, dx$$

where in case (A) the turning points are symmetric: $x = \pm a$; in case (B)—for the positive x well—the turning points are b and a.

Mathematica has problems doing the WKB integral directly:

```
Integrate[Sqrt[e-x^2(x^2-1)],{x,-a,a}]
```

Mathematica thinks for about 5 minutes but comes up with no answer. Gradshteyn & Ryzhik provides a result for the following equivalent integral (equivalent in the sense that we have a general quadratic in x^2 under a radical) and *Mathematica* can copy this result (it will take a few minutes):

```
Integrate[Sqrt[(c^2+x^2)(aa^2-x^2)],{x,-aa,aa}]
result=Simplify[%,{c>0,aa>0}]
Out[8]=(2*c*((aa - c)*(aa + c)*EllipticE[-(aa^2/c^2)] +
          (aa^2 + c^2)*EllipticK[-(aa^2/c^2)]))/3
```

The quartic under the root for the integral *Mathematica* can do is in factored form whereas our WKB integral is not; we have found the root a above, we need only express c in terms of E. If we compare the two:

$$(c^2 + x^2)(a^2 - x^2) = c^2a^2 + (a^2 - c^2)x^2 - x^4 = E - x^2(x^2 - 1) = E + x^2 - x^4$$

we conclude $c = \sqrt{E}/a$.

```
wkbA[e_]=alpha * result /. {c->Sqrt[e]/a,aa->a}
Plot[wkbA[e]/Pi,{e,0,.25}]
```

Now when the WKB integral equals $\pi(n - \frac{1}{2})$ we have a WKB solution. You can graphically find those spots from the graph of the integral as a function of `e`. For example $n - \frac{1}{2} = 19.5$; looking on the graph what E produces 19.5, I conclude near $E = .2$. I can then use *Mathematica* to improve that estimate:

```
FindRoot[wkbA[e]/Pi==19.5,{e,.2}]
Out[18]= {e -> 0.199938}
```

Problem: Graphically estimate the energy `e` for all n between 12 and 22 and then use `FindRoot` to produce accurate values. Put the results in a nice table.

For $E < 0$ the problem becomes more interesting as then we have two allowed regions separated by a disallowed region... the wavefunction will tunnel through that disallowed region and cover each equally. Since the problem is reflection symmetric the exact solutions will be either even or odd. Again, take a look at a low energy even/odd pair in `2well_all_psi.pdf`. So if we apply WKB to $E < 0$ it will only know about one well, and it will end up reporting the energy of what in fact turns out to be a pair of even/odd solutions. An additional irritant is that the *Mathematica* result for the factored WKB integral:

```
Integrate[Sqrt[(x^2-b^2)(a^2-x^2)],{x,b,a}]
```

includes and explicit `I` (i.e., looks complex, but is of course real). Gradshteyn & Ryzhik come to our rescue and report that this integral is:

```
wkbB[e_]=alpha*(a*((b^2+a^2)*EllipticE[(a^2-b^2)/a^2]-
           2*b^2*EllipticK[(a^2-b^2)/a^2]))/3
Plot[wkbB[e]/Pi,{e,-.25,0}]
```

Each of the five WKB energies you can determine from `wkbB[e]/Pi` correspond to a even/odd nearly degenerate pair; thus ten total eigenstates. Note: the 11^{th} eigenstate is too close to the boundary; you will find it neither in `wkbB[e]/Pi` (where the $E = 0$ value is about 5.4) or `wkbA[e]/Pi` (where the $E = 0$ value is about 10.9). Note 2: Griffiths 8.15 aims to improve these guesses, by using WKB to estimate the energy difference between the pair of nearly degenerate even & odd wavefunctions.

Problem: Graphically estimate the energy `e` for n between 1 and 5 and then use `FindRoot` to produce accurate values. Put the results in a nice table, noting that because they represent an even/odd nearly degenerate pair they actually constitute 10 eigenenergies. For the record the exact eigenenergy of the $n = 11$ state is $-.00176$.

FYI: These WKB energies deviate on average from the exact values by less than .0003!