

The potential

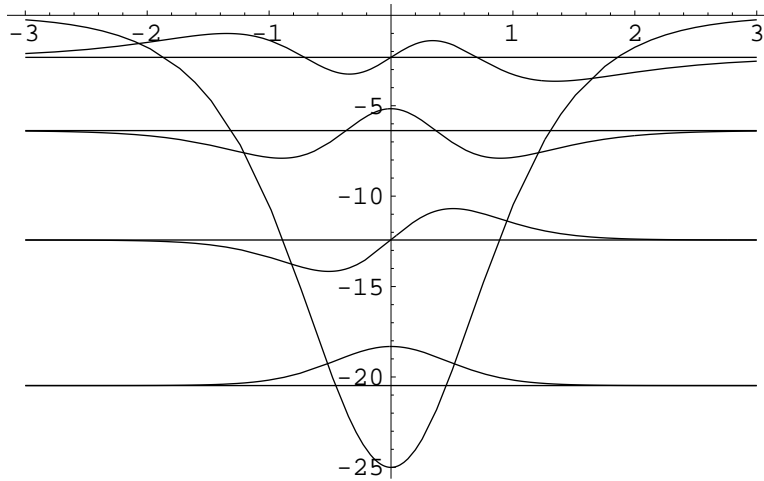
$$V(x) = -\frac{V_0}{\cosh^2(x/a)}$$

is exactly solvable and so provides a test case for various approximation methods. First as usual go to dimensionless coordinates with unit length  $l = a$  and unit energy  $e = \hbar^2/(2ma^2)$ :

$$\begin{aligned} \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi - \frac{V_0}{\cosh^2(x/a)} \psi &= E\psi \\ \frac{-\hbar^2}{2ma^2} \frac{\partial^2}{\partial x'^2} \psi - \frac{V_0}{\cosh^2(x')} \psi &= E\psi \\ -\frac{\partial^2}{\partial x'^2} \psi - \frac{V_0'}{\cosh^2(x')} \psi &= E'\psi \end{aligned}$$

(As usual on the following pages we will simplify by not writing the primes.) Note that the potential resembles a finite square well in that as  $|x| \rightarrow \infty$  the potential approaches zero. There are only a finite number of bound states ( $E < 0$ ) in addition to the continuum of free ( $E > 0$ ) states. Note that as  $|x| \rightarrow 0$  the potential looks quadratic, and so the low-energy solutions should look like SHO solutions (e.g., in having equally spaced eigenenergies).

Here is a stacked-wavefunction plot showing the four lowest states for  $V_0' = 25$ :



The exact eigenenergies are given by:

$$E'_n = -\left[\sqrt{V_0' + \frac{1}{4}} - \left(n + \frac{1}{2}\right)\right]^2$$

for  $n = 0$  up to the maximum value of  $n$  for which the value in square brackets ( $[ ]$ ) is positive.

1. Use the Rayleigh-Ritz (variational) method to estimate the eigenenergy of the ground state and first excited state for  $V_0 = 25$ . Use the trial wavefunctions:

$$\begin{aligned}\psi_0 &= \cosh(x) \exp(-qx^2) \\ \psi_1 &= x \cosh(x) \exp(-qx^2)\end{aligned}$$

Why are these reasonable choices? (Words please!) You will need to use *Mathematica* to do the integrals. Since you have symmetry, you might as well integrate only over the range  $[0, \infty]$ :

```
$Assumptions=$Assumptions && {q>1}
f[x_]=Cosh[x] Exp[- q x^2]
ke=Integrate[f'[x]^2,{x,0,Infinity}]
pe=-25 Integrate[f[x]^2/Cosh[x]^2,{x,0,Infinity}]
n=Integrate[f[x]^2,{x,0,Infinity}]
e=(ke+pe)/n
```

(The first line is to convince *Mathematica* that the integral actually converges. . . if  $q < 0$  the integrand would blow up as  $|x| \rightarrow \infty$ .) Use the *Mathematica* function `FindMinimum` to do the minimization:

```
FindMinimum[e,{q,your guess here}]
```

Note that you must give *Mathematica* a starting guess for  $q$ . I'd plot  $E$  vs.  $q$  to find a good guess for the minimum.

Compare your estimates to the exact eigenenergy given above. Plot both normalized wavefunctions using code similar to:

```
Plot[Evaluate[f[x]/Sqrt[n] /. q->your result here],{x,-2,2}]
```

2. Use the Rayleigh-Ritz (variational) method to estimate the eigenenergy of the ground state and first excited state for  $V_0 = 25$ . Use the trial wavefunctions:

$$\begin{aligned}\psi_0 &= 1/\cosh^q(x) \\ \psi_1 &= \sinh(x)/\cosh^q(x)\end{aligned}$$

Why are these reasonable choices? (Words please!) These integrals are simple enough that pencil and paper may be easier than *Mathematica*. *Mathematica* will express some results in terms of the hypergeometric  ${}_2F_1$  whereas using the below, you can do better:

$$\int_0^\infty \cosh^{-2q}(x) dx = \frac{\sqrt{\pi}}{2} \frac{\Gamma(q)}{\Gamma(q + \frac{1}{2})}$$

So:

$$\frac{\langle \psi_0 | \cosh^{-2} | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} = \frac{\Gamma(q+1)/\Gamma(q+\frac{3}{2})}{\Gamma(q)/\Gamma(q+\frac{1}{2})} = \frac{q}{q+\frac{1}{2}} \quad \text{Since: } \Gamma(x+1) = x\Gamma(x) = x!$$

and

$$\sinh^2(x) = \cosh^2(x) - 1$$

Compare your estimates to the exact eigenenergy given above. What can you conclude? Plot both normalized wavefunctions as in #1.

3. Since the potential looks quadratic for  $x \sim 0$ , we should be able to approximate using SHO. Thus since:

$$\cosh^{-2}(y) = 1 - y^2 + \frac{2}{3}y^4 - \frac{17}{45}y^6 + \dots$$

we have:

$$\begin{aligned} \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi - \frac{V_0}{\cosh^2(x/a)} \psi &= E\psi \\ \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x'^2} \psi + \frac{V_0}{a^2} x^2 \psi - \frac{V_0 2}{3a^4} x^4 \psi &\approx (E + V_0)\psi \\ -A \frac{\partial^2}{\partial x^2} \psi + B x^2 \psi - B \frac{2}{3a^2} x^4 \psi &\approx (E + V_0)\psi \end{aligned}$$

Using the length scale:  $l = (A/B)^{\frac{1}{4}}$  and energy scale:  $e = (AB)^{\frac{1}{2}}$ , we have:

$$\begin{aligned} \frac{-A}{(A/B)^{\frac{1}{2}}} \frac{\partial^2}{\partial x'^2} \psi + B(A/B)^{\frac{1}{2}} x'^2 \psi - B(A/B)^{\frac{1}{2}} \frac{2l^2}{3a^2} x'^4 \psi &\approx (E + V_0)\psi \\ -\frac{\partial^2}{\partial x'^2} \psi + x'^2 \psi - \frac{2l^2}{3a^2} x'^4 \psi &\approx (E' + V'_0)\psi \\ H_0 \psi - \frac{2l^2}{3a^2} x'^4 \psi &\approx (E' + V'_0)\psi \end{aligned}$$

where  $H_0$  is the SHO Hamiltonian with eigenenergies  $E_n^{(0)} = (2n + 1)$ . Thus  $E' + V'_0 = (E + V_0)/e = 2n + 1$  or

$$E = -V_0 + \left( \frac{\hbar^2}{2ma^2} V_0 \right)^{\frac{1}{2}} (2n + 1)$$

Dividing through by  $\hbar^2/2ma^2$  to produce the dimensionless quantities introduced for the  $1/\cosh^2$  potential, we have:

$$E' = -V'_0 + (V'_0)^{\frac{1}{2}} (2n + 1)$$

Whereas the exact answer is:

$$E' = - \left[ \sqrt{V'_0 + \frac{1}{4}} - \left(n + \frac{1}{2}\right) \right]^2 = -(V'_0 + \frac{1}{4}) + \left(V'_0 + \frac{1}{4}\right)^{\frac{1}{2}} (2n + 1) - \left(n + \frac{1}{2}\right)^2$$

Use first order perturbation theory to find how the  $x^4$  term affects the eigenenergies. Use second order perturbation theory to find the effect on the ground state. Hint: remember your raising and lower operators!

4. If we make the  $1/\cosh^2$  potential very deep and very narrow then it should approximate a delta function potential. Since:

$$\begin{aligned}\int_0^\infty V(x) dx &= - \int_0^\infty V_0/\cosh^2(x/a) dx = -V_0a \int_0^\infty 1/\cosh^2(y) dy \\ &= -V_0a \int_0^\infty \tanh'(y) dy = -V_0a\end{aligned}$$

we can keep the delta function potential strength  $w = 2V_0a$  a constant as  $V_0 \rightarrow \infty$  and  $a \rightarrow 0$ . See if the limit of the  $1/\cosh^2$  potential ground-state eigenenergy agrees with the delta function potential results derived on the web. What happens to the other bound states? (Note: in the above equations  $V_0$  is the actual potential not the dimensionless  $V'_0$ )

5. Find the WKB approximation for these eigenenergies. Hint: change variables in the WKB integral to  $u = \sinh(x)$ , note closely the range of integration in  $u$  and use the fact:

$$\int_0^A \frac{\sqrt{A^2 - u^2}}{1 + u^2} du = \frac{\pi}{2} (\sqrt{1 + A^2} - 1)$$

P.S. For folks knowing contour integration: Prove the above integral for extra credit.