Variational (Rayleigh - Ritz) method:

for any function f, $E_{gs} \leq \dfrac{\langle f|H|f\rangle}{\langle f|f\rangle}$ gs = ground state

Consider a function with various adjustable parameters $f(a,b,c;x)$. Find values for those parameters that produce the smallest value of $\dfrac{\langle f|H|f\rangle}{\langle f|f\rangle} \equiv E(a,b,c)$

This will be a smaller upper limit to E_{gs}

Pf: expand f in eigenfunctions of H: $f = \sum c_i \phi_i$

$$\frac{\langle f|H|f\rangle}{\langle f|f\rangle} = \frac{\sum |c_i|^2 E_i}{\sum |c_j|^2} \quad ; \quad \text{weight}_i = \frac{|c_i|^2}{\sum |c_j|^2}$$

→ weighted avg of E_i must be bigger (or equal) to smallest $E_i = E_{gs}$

Note: Let $i=0$ be the ground state. If (for example) by symmetry we can know $c_0 = 0$ then $\dfrac{\langle f|H|f\rangle}{\langle f|f\rangle}$ is weighted avg of all but gs & so must be bigger (or equal) to smallest in remaining set — the first excited state.

"Quadratic accuracy" → if $f = \phi_i + \varepsilon g$ then

$$E(a,b,c) = \frac{\langle f|H|f\rangle}{\langle f|f\rangle} = \frac{E_i\left\{\langle \phi_i|\phi_i\rangle + \varepsilon\langle \phi_i|g\rangle + \varepsilon^*\langle g|\phi_i\rangle + E_i|\varepsilon|^2\langle g|g\rangle - E_i|\varepsilon|^2\langle g|g\rangle\right\} + |\varepsilon|^2\langle g|H|g\rangle}{\langle \phi_i|\phi_i\rangle + \varepsilon\langle \phi_i|g\rangle + \varepsilon^*\langle g|\phi_i\rangle + |\varepsilon|^2\langle g|g\rangle}$$

$$= E_i + \frac{|\varepsilon|^2\langle g|H - E_i|g\rangle}{\langle \phi_i|\phi_i\rangle + 2\,\mathrm{Re}\left[\varepsilon\langle \phi_i|g\rangle\right] + |\varepsilon|^2\langle g|g\rangle}$$

SHO gs $\quad \frac{-\hbar^2}{2m}\partial_x^2 + \frac{1}{2}m\omega^2 \qquad \psi = \begin{cases} (a^2-x^2) & |x|<a \\ 0 & |x|>a \end{cases}$

$KE = \frac{+\hbar^2}{2m}\int (\partial_x f)^2 dx = \frac{\hbar^2}{2m}\left\{ 2\int_0^a (2x)^2 dx = \frac{8}{3}a^3 \right\}$

$PE = \frac{1}{2}m\omega^2 \int \psi^2 x^2 dx = \frac{1}{2}m\omega^2 \left\{ 2\int_0^a \underbrace{(a^2-x^2)^2 x^2}_{a^4x^2 - 2a^2x^4 + x^6} dx = 2\left[\frac{1}{3}a^7 - \frac{2}{5}a^7 + \frac{a^7}{7}\right] \right. \to 16/105\, a^7$

$N = \int \psi^2 dx = 2\int_0^a \underbrace{(a^2-x^2)^2}_{a^4 - 2a^2x^2 + x^4} dx = 2\left[a^5 - \frac{2}{3}a^5 + \frac{1}{5}a^5\right] = \frac{16}{15}a^5$

$"E" = \frac{KE+PE}{N} = \frac{\frac{\hbar^2}{2m}\frac{8}{3}a^3 + \frac{1}{2}m\omega^2\frac{16}{105}a^7}{\frac{16}{15}a^5} = \frac{1}{2}\hbar\omega\left[\frac{\hbar}{m\omega}\frac{8}{3}a^{-2} + \frac{m\omega}{\hbar}\frac{16}{105}a^2\right]\frac{15}{16}$

call x

$= \frac{1}{2}\hbar\omega\left[\frac{8}{3}\frac{1}{x} + \frac{16}{105}x\right]\frac{15}{16}$

$\hookrightarrow$ minimize: $\frac{-8}{3}\frac{1}{x^2} + \frac{16}{105} = 0 \to x = \sqrt{\frac{8}{3}\cdot\frac{105}{16}}$

plug min x into [ ] $= 1.275 \times \frac{15}{16} \Rightarrow \underline{1.20}$

our upperbound on E_{gs} is 20% above actual.

use Mathematica with $\psi = \frac{1}{\cosh(ax)}$

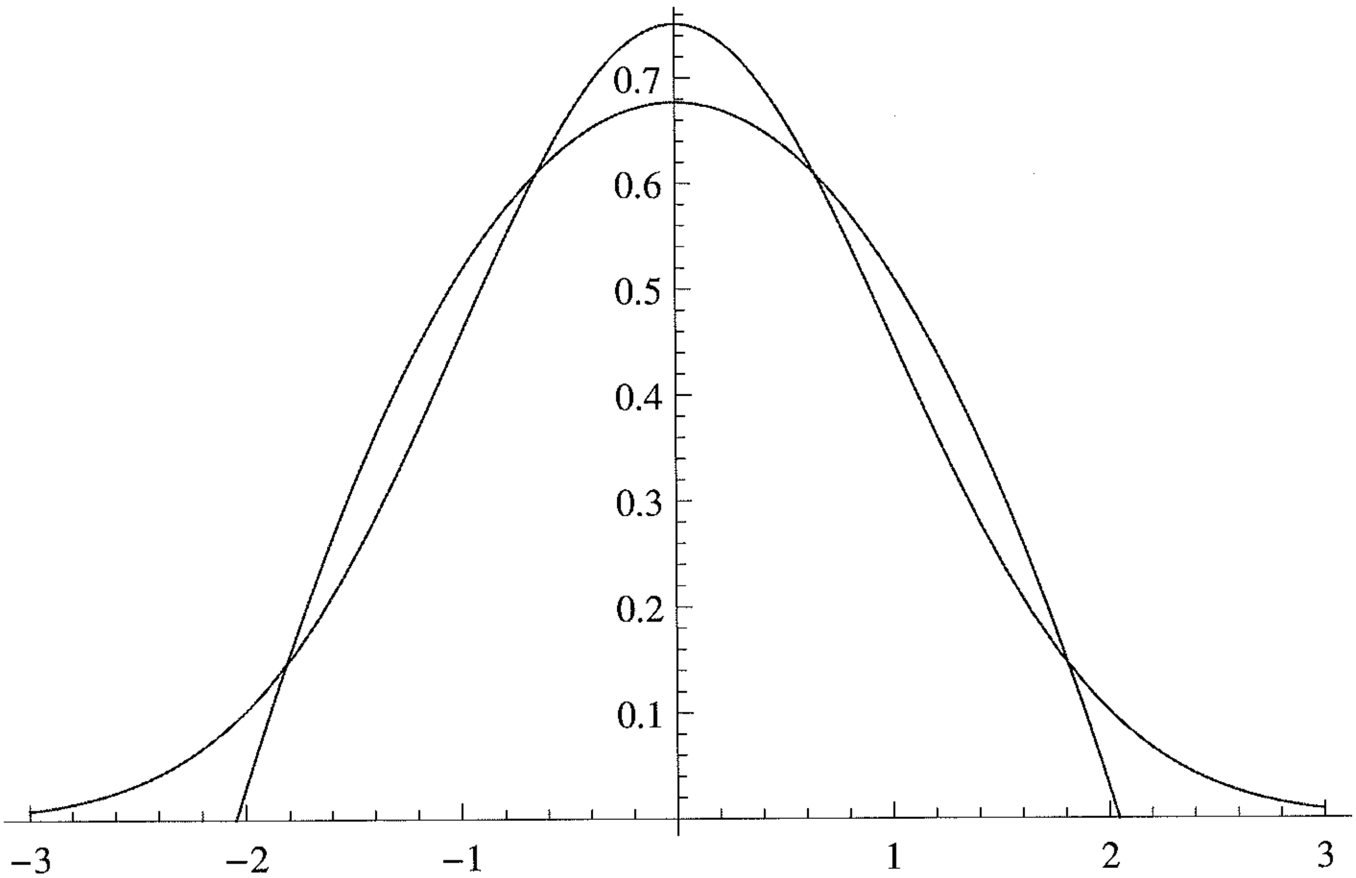
$\int (\partial_x\psi)^2 dx = \frac{2}{3}a \qquad \int \psi^2 x^2 = \frac{\pi^2}{6a^3} \qquad \int \psi^2 dx = \frac{2}{a}$

$"E" = \frac{KE+PE}{N} = \frac{\frac{\hbar^2}{2m}\frac{2}{3}a + \frac{1}{2}m\omega^2\frac{\pi^2}{6a^3}}{\frac{2}{a}} = \frac{\hbar\omega}{2}\left[\frac{\hbar}{m\omega}\frac{1}{3}a^2 + \frac{m\omega}{\hbar}\frac{\pi^2}{12a^2}\right]$

call x

$= \frac{\hbar\omega}{2}\left[\frac{1}{3}x + \frac{\pi^2}{12}\frac{1}{x}\right]$

min: $\frac{1}{3} - \frac{\pi^2}{12x^2} = 0 \qquad x = \frac{\pi}{2} \qquad [\,] = 1.05$



0.7
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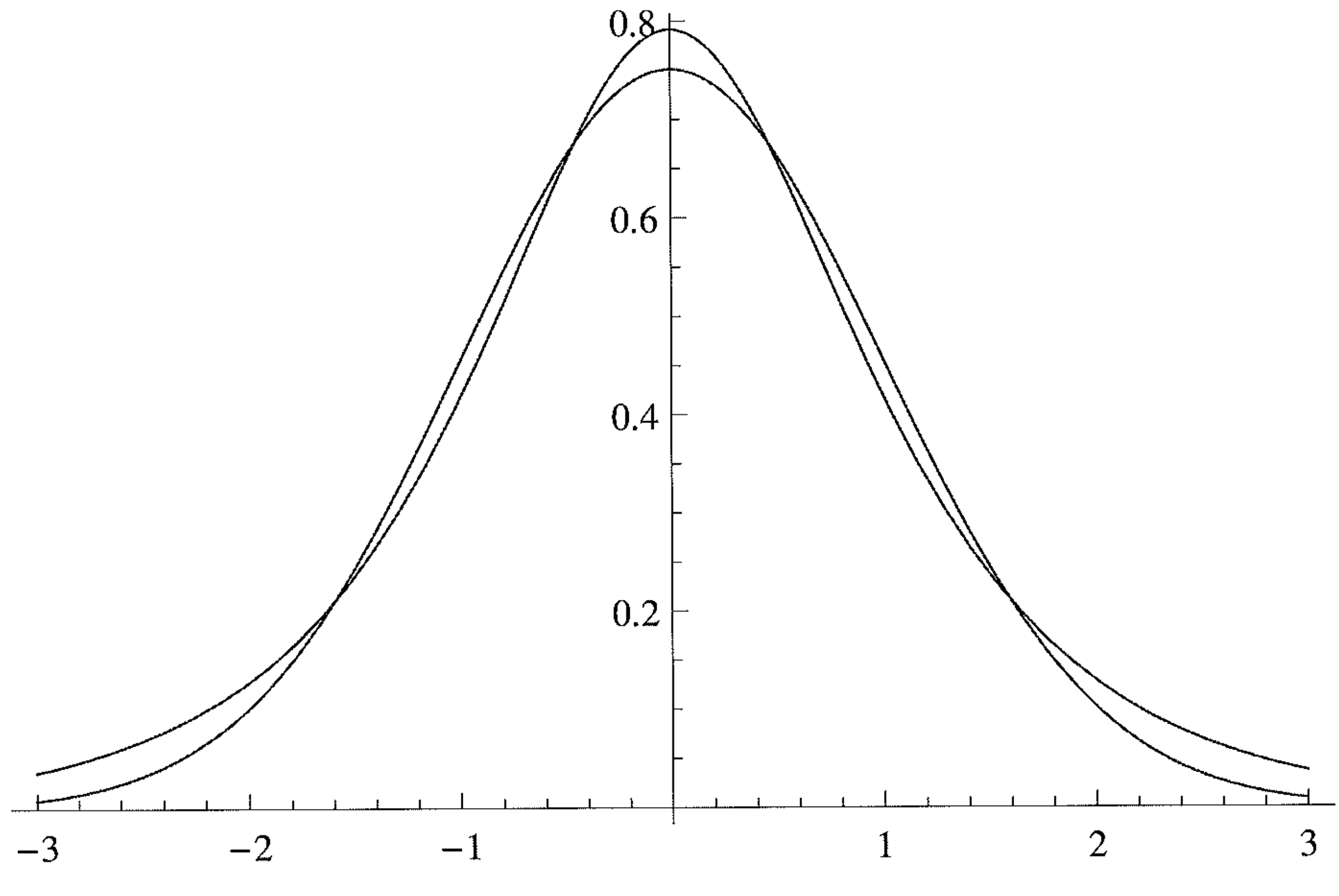


0.8
0.6
0.4
0.2
−3
−2
−1
1
2
3

```
$Assumptions=$Assumptions && {a>0}
f[x_]=1/Cosh[a x]
ke=Integrate[f'[x]^2,{x,-Infinity,Infinity}]
          2 a
Out[3]= ---
           3

pe=Integrate[x^2 f[x]^2,{x,-Infinity,Infinity}]
            2
          Pi
Out[4]= ----
              3
          6 a

n=Integrate[f[x]^2,{x,-Infinity,Infinity}]
          2
Out[5]= -
          a
```

Symmetric trial

```
f[x_]=Exp[-a (x-2)^2]+Exp[-a (x+2)^2]

ke=Integrate[f'[x]^2,{x,-Infinity,Infinity}]
                                    8 a
          Sqrt[a] (1 - 16 a + E    ) Sqrt[2 Pi]
Out[7]= ------------------------------------
                               8 a
                              E

pe=-2(1+Exp[-a 4^2])
direct=0, exchange=-Exp[-a 4^2], self=-1
n=Integrate[f[x]^2,{x,-Infinity,Infinity}]
                  8 a
          (1 + E    ) Sqrt[2 Pi]
Out[9]= ---------------------
                         8 a
               Sqrt[a] E

(ke/2+pe)/n
Plot[%,{a,.1,2}]
FindMinimum[%%,{a,.5}]
Out[12]= {-0.340238, {a -> 0.490313}}
```

antisym trial

```
f[x_]=Exp[-a (x-2)^2]-Exp[-a (x+2)^2]
ke=Integrate[f'[x]^2,{x,-Infinity,Infinity}]
                                      8 a
           Sqrt[a] (-1 + 16 a + E    ) Sqrt[2 Pi]
Out[15]= -------------------------------------
                                 8 a
                                E
pe=-2(1-Exp[-a 4^2])
direct=0, exchange=+Exp[-a 4^2], self=-1
n=Integrate[f[x]^2,{x,-Infinity,Infinity}]
                   8 a
           (-1 + E    ) Sqrt[2 Pi]
Out[17]= ----------------------
                          8 a
                Sqrt[a] E

(ke/2+pe)/n
Plot[%,{a,.1,2}]
FindMinimum[%%,{a,.75}]
Out[20]= {-0.306583, {a -> 0.766212}}

exact: -0.480369 & -0.517251
```

vs -.307 -.340

δ function dimensionless
see delta.02.html

$$\left(-\underbrace{\frac{\hbar^2}{2m}}_{\text{"A" = units } E\cdot L^2}\partial_x^2 + w\,\delta(x-a)\right)\psi = E\psi$$

units: E·L

Length = $\frac{A}{w}$ = ℓ Energy = w^2/A = e

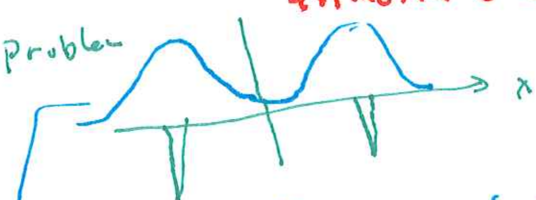
$$\left(-\frac{\hbar^2}{2m\ell^2}\partial_{x'}^2 + \frac{w}{\ell}\delta(x'-a')\right)\psi = E' e\,\psi$$

w^2/A w^2/A w^2/A

$$\left(-\frac{1}{2}\partial_{x'}^2 + \delta(x'-a')\right)\psi = E'\psi$$

attractive δ at $x' = \pm 2$

problem



trial wf: sum of gaussians at $x = \pm 2$

$e^{-a(x+2)^2} + e^{-a(x-2)^2}$

Complete no more than 5 of the following problems

1. (R-R) Consider the problem of two attractive delta function potentials symmetrically located about the origin at $x = \pm a$, with dimensionless Hamiltonian:

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x)$$

where

$$V(x) = -[\delta(x-a) + \delta(x+a)]$$

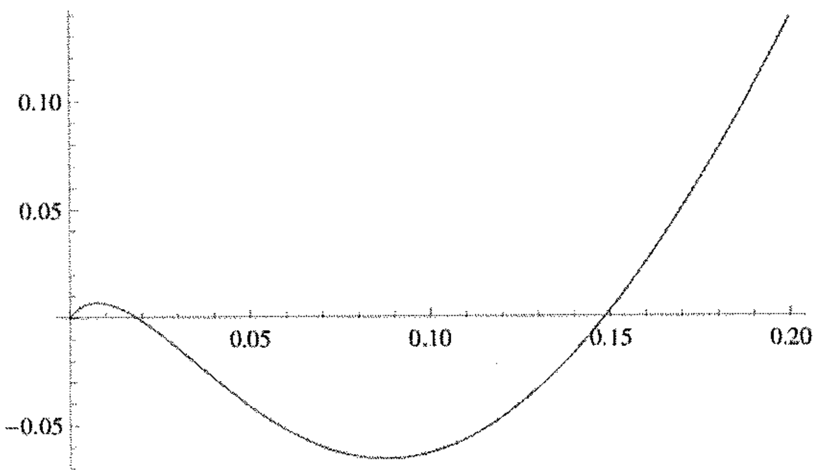
The trial function $f(x) = xe^{-bx^2}$ is used to evaluate $\langle H \rangle = \langle f|H|f\rangle / \langle f|f\rangle$:

(a) Calculate: $\langle f|V(x)|f\rangle$

(b) Calculate $\langle f|f\rangle$ (You may find the integrals on the cheat sheet helpful.)

(c) The below plot shows $\langle H \rangle$ plotted as a function of $b \in [0, .2]$ for $a = 2$. Use this graph to make as precise statement as you can about the exact eigenenergies of this system.

(d) Suggest a trial wavefunction to approximate the ground state of this system.

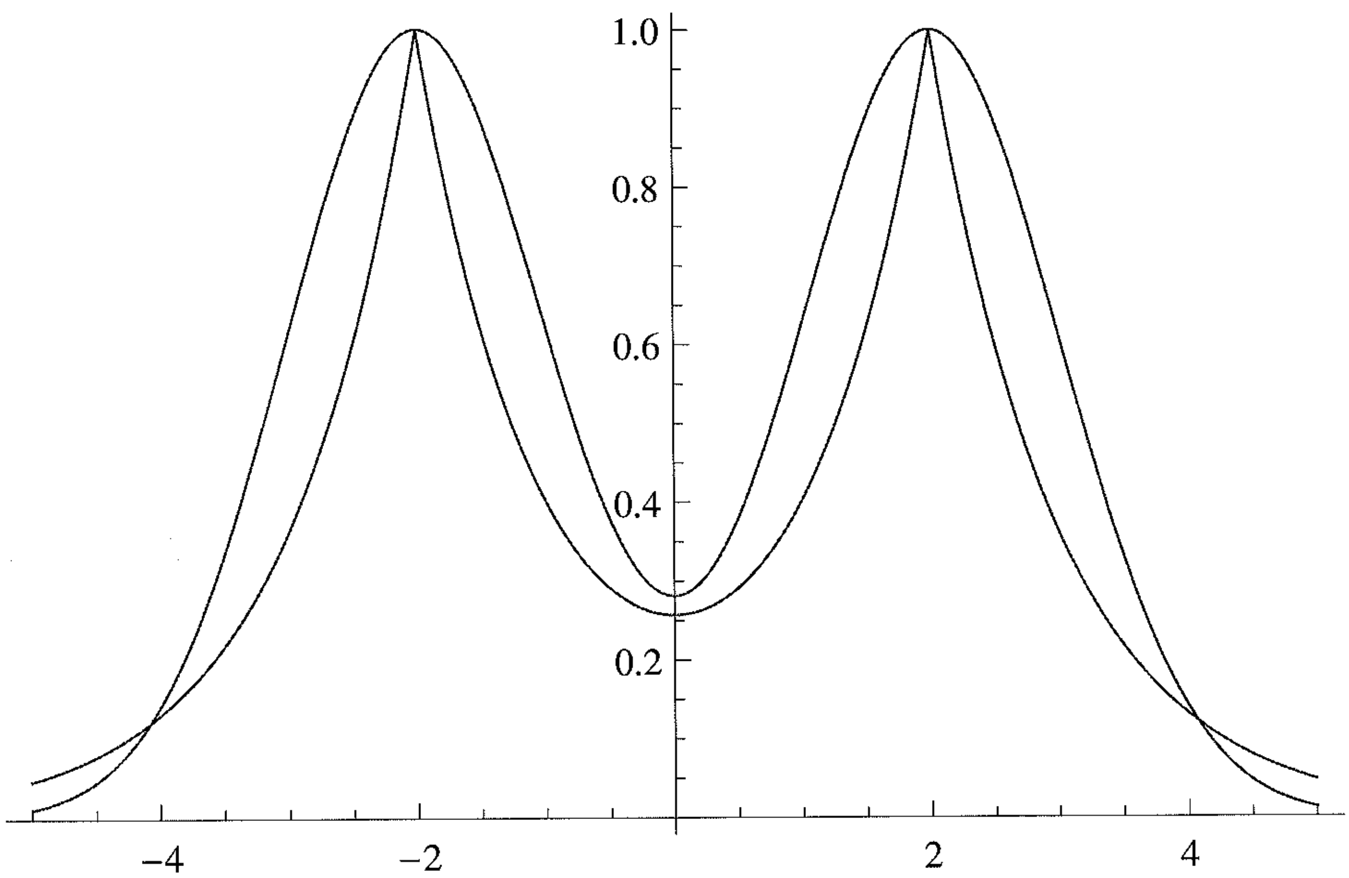


2. (R-R) The ground state energy of a system is estimated both by the Rayleigh-Ritz method and by a second-order perturbation theory calculation. The Rayleigh-Ritz result is −27.1 eV; the perturbation theory result is −26.0 eV. Which lies closer to the true ground state energy? Why? What is required for the R-R method to give an accurate bound for an excited state?

3. (WKB+) Consider the potential

$$V(x) = \lambda\,|x|$$

where λ is a positive constant. Provide rough sketches the three lowest energy eigenfunctions. Label the ground state ψ_1, the first excited state ψ_2, etc. Consider the symmetry of these three states: record which state(s) are even, odd, or of no definite symmetry. Some integrals must zero simply because of symmetry. Which (if any) of the following integrals are zero because of symmetry: $\langle\psi_2|\psi_2\rangle$, $\langle\psi_1|\psi_2\rangle$, $\langle\psi_3|x|\psi_1\rangle$, $\langle\psi_3|x|\psi_2\rangle$, and $\langle\psi_1|\frac{d}{dx}|\psi_2\rangle$. Sketch a large n wavefunction (ψ_n), being careful to show wavefunction behavior (x variation of amplitude and wavelength) as required by WKB.



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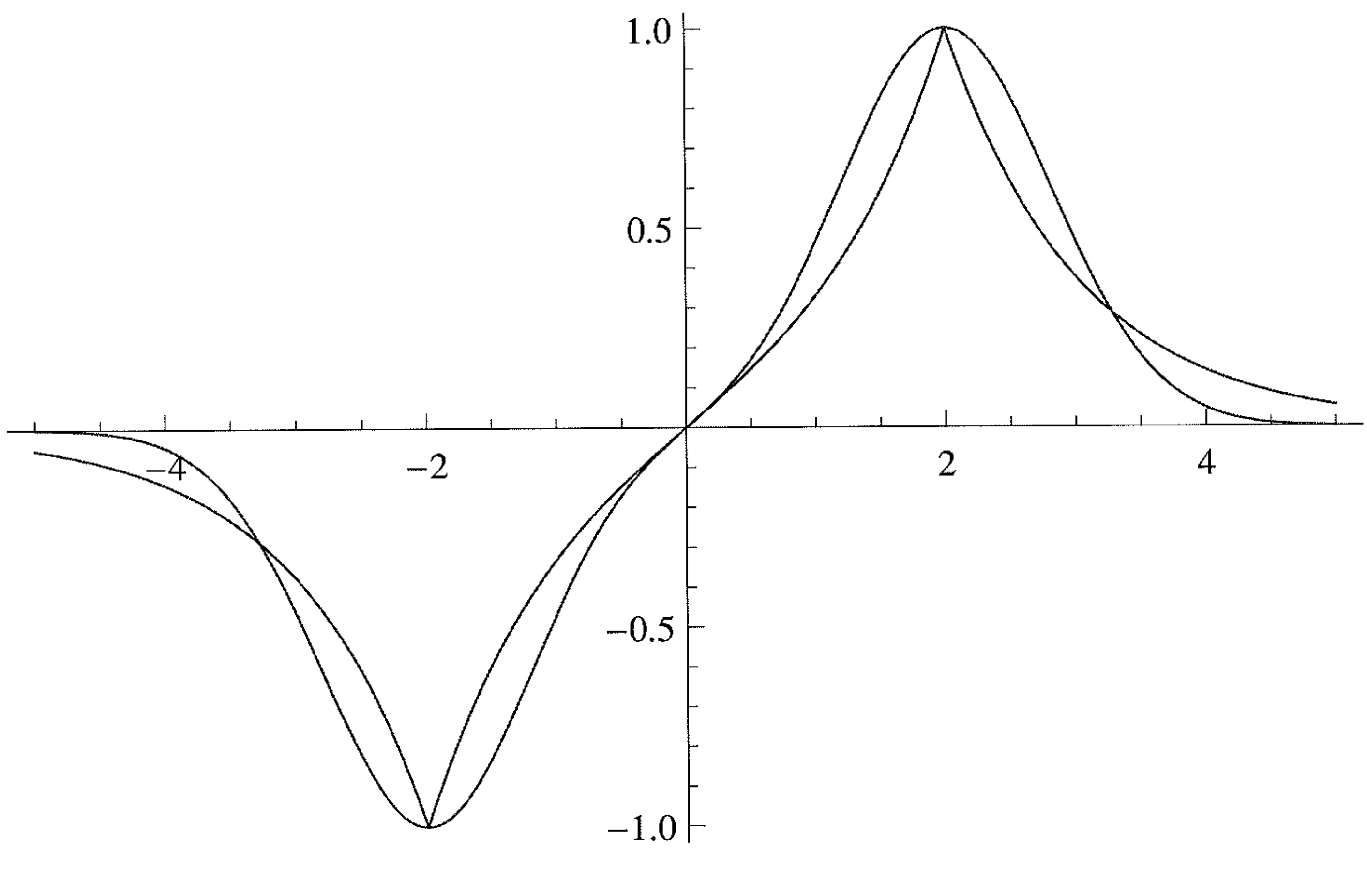

1.0
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−1.0