HW 8-1 pb 4

November 3, 2025

Input:

```
(* Infinite Square Well - Variational Method *) (* Merzbacher Problem 8.1
   - Complete Solution *) (* Pure symbolic version - no numerical
   substitution *) Clear [ "\<Global`*\>" ] $Assumptions = a > 0 && b > 0
   ; \
Print [ "\<\>" ] Print [ "\<INFINITE␣SQUARE␣WELL␣VARIATIONAL␣CALCULATION\>
   " ] Print [ ] Print [ "\<Boundary␣conditions:␣[Psi]([PlusMinus]a)␣=␣0\>
   " ] Print [ "\<\>" ] \
(* === === === === === === === === === === === === === === === === === === ===
    === === === === === === *) \
Print [ "\<\>" ] Print [ "\<PART␣(a):␣TRAPEZOIDAL␣TRIAL␣FUNCTION\>" ]
   Print [ "\<\>" ] \
Print [ "\<Trial␣function:\>" ] Print [ ] Print [ ] Print [ "\<\>" ] \
Print [ "\<Case␣(i):␣b␣=␣0␣(Triangular␣function)\>" ] Print [ "\<\>" ] \
Print [ "\<Normalization␣integral:\>" ] Print [ "\<␣N␣=␣[Integral]_{-a}^{a
   }␣(a␣-␣|x|)^2␣dx\>" ] Print [ ] Print [ ] Print [ "\<␣=␣[a^2␣x␣-␣ax^2␣+
   ␣x^3/3]_{0}^{a}\>" ] Print [ "\<␣=␣a^3␣-␣a^3␣+␣a^3/3\>" ] Print [ "\<␣=
   ␣a^3/3\>" ] normIntTri = Simplify [ 2 * Integrate [ ( a - x ) ^ 2 , { x
    , 0 , a } ] ] Print [ "\<␣N␣=␣\>" , normIntTri ] \
ATri = Simplify [ 1 / Sqrt [ normIntTri ] ] Print [ "\<␣A␣=␣1/[Sqrt]N␣=␣\>
   " , ATri ] Print [ "\<\>" ] \
Print [ "\<Kinetic␣energy␣calculation:\>" ] Print [ "\<␣d[Psi]/dx␣=␣-A␣for
   ␣0␣<␣x␣<␣a\>" ] Print [ "\<␣d[Psi]/dx␣=␣+A␣for␣-a␣<␣x␣<␣0\>" ] Print [
   ] Print [ ] Print [ "\<␣=␣([HBar]^2/2m)␣[Times]␣2A^2␣a\>" ] kineticTri
   = Simplify [ 2 * Integrate [ ATri ^ 2 , { x , 0 , a } ] ] Print [ "\<␣=
   ␣([HBar]^2/2m)␣[Times]␣\>" , kineticTri ] Print [ "\<␣<E>␣=␣([HBar]^2/2
   m)␣[Times]␣\>" , Simplify [ kineticTri / a ^ 2 ] , "\</a^2\>" ] Print [
    "\<\>" ] \
Print [ Framed [ Style [ "\<ANSWER␣(Case␣i):␣<E>␣=␣\>" <> ToString [
   Simplify [ kineticTri / a ^ 2 ] , TraditionalForm ] <> "\<␣[HBar]^2/(2
   ma^2)\>" , , 14 ] , FrameStyle -> Thick , Background -> LightYellow ] ]
    Print [ "\<\>" ] \
Print [ "\<Case␣(ii):␣Optimize␣parameter␣b\>" ] Print [ "\<\>" ] \
Print [ "\<Normalization␣integral:\>" ] Print [ "\<␣N␣=␣[Integral]_{-a}^{a
   }␣[Psi]^2␣dx\>" ] Print [ ] Print [ "\<␣By␣symmetry␣of␣outer␣regions:\>
   " ] Print [ ] Print [ "\<␣=␣2[(a␣-␣x)^3/(-3)]_{b}^{a}␣+␣2b(a␣-␣b)^2\>"
   ] Print [ "\<␣=␣2(a␣-␣b)^3/3␣+␣2b(a␣-␣b)^2\>" ] part1 = Integrate [ ( a
    - x ) ^ 2 , { x , b , a } ] part2 = Integrate [ ( a - b ) ^ 2 , { x ,
   - b , b } ] normTrap = Simplify [ 2 * part1 + part2 ] Print [ "\<␣N(b)␣
   =␣\>" , normTrap ] Print [ "\<\>" ] \
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ATrap = 1 / Sqrt [ normTrap ] Print [ "\<Kinetic energy calculation:\>" ]
   Print [ ] Print [ "\< d[Psi]/dx = -1 for b < x < a\>" ] Print [ "\< d[
   Psi]/dx = +1 for -a < x < -b\>" ] Print [ ] Print [ "\< = ([HBar]^2/2m)
   [Times]2(a - b)/N\>" ] kineticTrap = Simplify [ 2 * Integrate [ ATrap
    ^ 2 , { x , b , a } ] ] Print [ "\< = ([HBar]^2/2m)[Times]\>" ,
   kineticTrap ] Print [ "\<\>" ] \
dEdb = Simplify [ D [ kineticTrap , b ] ] Print [ "\<Optimization:\>" ]
   Print [ "\< d<E>/db = ([HBar]^2/2m)[Times]\>" , dEdb ] Print [ "\<\>"
    ] Print [ ] Print [ ] Print [ "\<\>" ] \
Print [ Framed [ Style [ , , 14 ] , FrameStyle -> Thick , Background ->
   LightYellow ] ] Print [ "\<\>" ] \
(* === === === === === === === === === === === === === === === === === === ===
    === === === === === === *) \
Print [ "\<\>" ] Print [ "\<PART (b): PARABOLIC TRIAL FUNCTION\>" ] Print
   [ "\<\>" ] \
Print [ ] Print [ "\<\>" ] \
Print [ "\<Normalization integral:\>" ] Print [ "\< N = [Integral]_{-a}^{a
   }(x^2 - a^2)^2 dx\>" ] Print [ "\< = [Integral]_{-a}^{a}(x^4 - 2a^2 x
   ^2 + a^4) dx\>" ] Print [ "\< By symmetry (all terms are even):\>" ]
   Print [ "\< = 2[Integral]_{0}^{a}(x^4 - 2a^2 x^2 + a^4) dx\>" ] Print
   [ "\< = 2[x^5/5 - 2a^2 x^3/3 + a^4 x]_{0}^{a}\>" ] Print [ "\< = 2(a
   ^5/5 - 2a^5/3 + a^5)\>" ] Print [ "\< = 2a^5(1/5 - 2/3 + 1)\>" ] Print
   [ "\< = 2a^5(3/15 - 10/15 + 15/15)\>" ] Print [ "\< = 2a^5(8/15)\>" ]
   normIntB = Integrate [ ( x ^ 2 - a ^ 2 ) ^ 2 , { x , - a , a } ] Print
   [ "\< N = \>" , normIntB ] \
AB = Simplify [ 1 / Sqrt [ normIntB ] ] Print [ "\< A = \>" , AB ] Print [
    "\<\>" ] \
Print [ "\<Derivative: d[Psi]/dx = 2Ax\>" ] Print [ "\<\>" ] \
Print [ "\<Kinetic energy calculation:\>" ] Print [ ] Print [ "\< = ([HBar
   ]^2/2m)[Integral]_{-a}^{a}(2Ax)^2 dx\>" ] Print [ ] Print [ "\< By
   symmetry:\>" ] Print [ ] Print [ "\< = ([HBar]^2/2m)[Times]8A^2[x
   ^3/3]_{0}^{a}\>" ] Print [ "\< = ([HBar]^2/2m)[Times]8A^2a^3/3\>" ]
   kineticIntB = Integrate [ ( 2 * AB * x ) ^ 2 , { x , - a , a } ]
   kineticIntB = Simplify [ kineticIntB ] Print [ "\< = ([HBar]^2/2m)[
   Times]\>" , kineticIntB ] Print [ "\< <E> = ([HBar]^2/2m)[Times]\>"
   , Simplify [ kineticIntB / a ^ 2 ] , "\</a^2\>" ] Print [ "\<\>" ] \
Print [ Framed [ Style [ "\<ANSWER (Part b): <E> = \>" <> ToString [
   Simplify [ kineticIntB / a ^ 2 ] , TraditionalForm ] <> "\< [HBar]^2/(2
   ma^2)\>" , , 14 ] , FrameStyle -> Thick , Background -> LightYellow ] ]
    Print [ "\<\>" ] \
(* === === === === === === === === === === === === === === === === === === ===
    === === === === === === *) \
Print [ "\<\>" ] Print [ "\<PART (c): QUARTIC TRIAL FUNCTION\>" ] Print [
   "\<\>" ] \
Print [ ] Print [ "\<Variational parameter: r = [Alpha]/[Beta]\>" ] Print
   [ "\<\>" ] \
[Psi]cFunc [ x_ ] := ( a ^ 2 - x ^ 2 ) * ( [Alpha] * x ^ 2 + [Beta] )
   Print [ ] Print [ "\<\>" ] \
Print [ "\<Normalization integral:\>" ] Print [ ] Print [ ] Print [ ]
   normIntC = Integrate [ [Psi]cFunc [ x ] ^ 2 , { x , - a , a } ]
   normIntC = Simplify [ normIntC ] Print [ "\< N = \>" , normIntC ] Print
    [ "\<\>" ] \
AC = 1 / Sqrt [ normIntC ] \
Print [ "\<Derivative calculation:\>" ] Print [ ] Print [ ] Print [ ]
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    Print [ ] Print [ "\<␣=␣2[Alpha]a^2␣x␣-␣4[Alpha]x^3␣-␣2[Beta]x\>" ] d[
    Psi]cFunc = D [ [Psi]cFunc [ x ] , x ] Print [ "\<␣d[Psi]/dx␣=␣\>" , d[
    Psi]cFunc ] Print [ "\<\>" ] \
Print [ "\<Kinetic␣energy␣integral:\>" ] Print [ ] Print [ ] Print [ "\<␣(
    Even␣function␣integrated␣over␣symmetric␣limits)\>" ] kineticIntCNum =
    Integrate [ d[Psi]cFunc ^ 2 , { x , - a , a } ] kineticIntCNum =
    Simplify [ kineticIntCNum ] Print [ "\<␣Numerator␣=␣\>" ,
    kineticIntCNum ] Print [ "\<\>" ] \
kineticIntC = Simplify [ kineticIntCNum / normIntC ] Print [ "\<␣<T>␣=␣([
    HBar]^2/2m)␣[Times]␣\>" , kineticIntC ] Print [ "\<\>" ] \
energyC = Simplify [ kineticIntC /. [Alpha] -> r * [Beta] ] Print [ "\<
    Energy␣as␣function␣of␣r␣=␣[Alpha]/[Beta]:\>" ] Print [ "\<␣<E>(r)␣=␣([
    HBar]^2/2m)␣[Times]␣\>" , energyC ] Print [ "\<\>" ] \
dEdr = Simplify [ D [ energyC , r ] ] Print [ "\<Variational␣condition␣d<E
    >/dr␣=␣0:\>" ] Print [ "\<␣d<E>/dr␣=␣([HBar]^2/2m)␣[Times]␣\>" , dEdr ]
     Print [ "\<\>" ] \
rSols = Solve [ dEdr == 0 , r ] Print [ "\<Solutions␣for␣optimal␣r:\>" ]
    r1 = Simplify [ r /. rSols [ [ 1 ] ] ] r2 = Simplify [ r /. rSols [ [ 2
     ] ] ] Print [ "\<␣r\[Subscript␣1]␣=␣\>" , r1 ] Print [ "\<␣r\[
    Subscript␣2]␣=␣\>" , r2 ] Print [ "\<\>" ] \
E1 = Simplify [ energyC /. r -> r1 ] E2 = Simplify [ energyC /. r -> r2 ]
    \
Print [ "\<Energy␣values:\>" ] Print [ "\<␣At␣r\[Subscript␣1]:␣<E>␣=␣([
    HBar]^2/2m)␣[Times]␣\>" , Simplify [ E1 / a ^ 2 ] , "\</a^2\>" ] Print
    [ "\<␣At␣r\[Subscript␣2]:␣<E>␣=␣([HBar]^2/2m)␣[Times]␣\>" , Simplify [
    E2 / a ^ 2 ] , "\</a^2\>" ] Print [ "\<\>" ] \
(* Compare which is smaller *) \
E1num = N [ E1 /. a -> 1 ] E2num = N [ E2 /. a -> 1 ] \
If [ E1num < E2num , Print [ "\<Selecting␣r\[Subscript␣1]␣(minimum␣energy)
    \>" ] ; \
rOpt = r1 ; energyCOpt = E1 , Print [ "\<Selecting␣r\[Subscript␣2]␣(
    minimum␣energy)\>" ] ; \
rOpt = r2 ; energyCOpt = E2 ] \
Print [ "\<\>" ] Print [ "\<Optimal␣parameters:\>" ] Print [ "\<␣r\[
    Subscript␣opt]␣=␣\>" , rOpt ] Print [ "\<␣<E>␣=␣([HBar]^2/2m)␣[Times]␣
    \>" , Simplify [ energyCOpt / a ^ 2 ] , "\</a^2\>" ] Print [ "\<\>" ] \
Print [ Framed [ Column [ { Style [ "\<ANSWER␣(Part␣c):\>" , , 14 ] ,
    Style [ "\<Optimal␣r␣=␣\>" <> ToString [ rOpt , TraditionalForm ] , ,
    12 ] , Style [ "\<<E>␣=␣\>" <> ToString [ Simplify [ energyCOpt / a ^ 2
     ] , TraditionalForm ] <> "\<␣[HBar]^2/(2ma^2)\>" , , 12 ] } ] ,
    FrameStyle -> Thick , Background -> LightYellow ] ] Print [ "\<\>" ] \
(* === === === === === === === === === === === === === === === === === ===
     === === === === === === *) \
Print [ "\<\>" ] Print [ "\<PART␣(d):␣COMPARISON␣WITH␣EXACT␣RESULT\>" ]
    Print [ "\<\>" ] \
exactEnergy = [Pi] ^ 2 / ( 8 * a ^ 2 ) \
Print [ "\<Exact␣ground␣state:\>" ] Print [ ] Print [ , exactEnergy ]
    Print [ "\<\>" ] \
Print [ "\<Summary␣of␣Variational␣Estimates\>" ] Print [ "\<\>" ] \
Print [ Style [ , ] ] Print [ "\<Exact␣\>" , exactEnergy ] Print [ "\<
    Triangular␣\>" , Simplify [ kineticTri / a ^ 2 ] ] Print [ "\<Parabolic
    ␣\>" , Simplify [ kineticIntB / a ^ 2 ] ] Print [ "\<Quartic␣(optimized
    )␣\>" , Simplify [ energyCOpt / a ^ 2 ] ] Print [ "\<\>" ] \
Print [ ] Print [ "\<Triangular:␣\>" , N [ Simplify [ kineticTri / a ^ 2 ]
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    /. a -> 1 ] , "\<␣[GreaterEqual]␣\>" , N [ [Pi] ^ 2 / 8 ] , "\<␣[
   Checkmark]\>" ] Print [ "\<Parabolic:␣\>" , N [ Simplify [ kineticIntB
   / a ^ 2 ] /. a -> 1 ] , "\<␣[GreaterEqual]␣\>" , N [ [Pi] ^ 2 / 8 ] , "
   \<␣[Checkmark]\>" ] Print [ "\<Quartic:␣\>" , N [ Simplify [ energyCOpt
    / a ^ 2 ] /. a -> 1 ] , "\<␣[GreaterEqual]␣\>" , N [ [Pi] ^ 2 / 8 ] ,
   "\<␣[Checkmark]\>" ] Print [ "\<\>" ] \
Print [ Framed [ Column [ { Style [ "\<ANSWER␣(Part␣d):\>" , , 14 ] ,
   Style [ , , 12 ] , Style [ , , 12 ] } ] , FrameStyle -> Thick ,
   Background -> LightYellow ] ] Print [ "\<\>" ] \
Print [ "\<Mean-Square␣Deviations\>" ] Print [ "\<\>" ] \
Print [ ] Print [ "\<\>" ] \
(* Symbolic overlap integrals *) \
[Psi]0Sym [ x_ ] := ( 1 / Sqrt [ a ] ) * Cos [ [Pi] * x / ( 2 * a ) ] [Psi
   ]bSym [ x_ ] := AB * ( x ^ 2 - a ^ 2 ) \
Print [ "\<Parabolic␣function:\>" ] overlapBSym = Integrate [ [Psi]0Sym [
   x ] * [Psi]bSym [ x ] , { x , - a , a } ] overlapBSym = Simplify [
   overlapBSym ] Print [ , overlapBSym ] msdBSym = Simplify [ 2 * ( 1 -
   overlapBSym ) ] Print [ "\<␣Mean-square␣deviation:␣[CapitalDelta]^2␣=␣
   \>" , msdBSym ] Print [ "\<\>" ] \
Print [ ] Print [ "\<\>" ] \
(* === === === === === === === === === === === === === === === === === === ===
    === === === === === === *) \
Print [ "\<\>" ] Print [ ] Print [ "\<\>" ] \
Print [ , rOpt ] Print [ "\<\>" ] \
Print [ "\<Nodes␣occur␣at:\>" ] Print [ ] Print [ ] Print [ "\<\>" ] \
Print [ "\<Interior␣node␣condition:␣x^2␣=␣-1/r␣=␣\>" , Simplify [ - 1 /
   rOpt ] ] \
rNum = N [ rOpt ] xSq = N [ - 1 / rNum ] \
If [ xSq > 0 , Print [ "\<Real␣interior␣nodes␣exist␣at␣x^2␣=␣\>" ,
   Simplify [ - 1 / rOpt ] ] ; \
If [ Simplify [ - 1 / rOpt ] < a ^ 2 , Print [ "\<Location:␣INSIDE␣the␣
   well␣(|x|␣<␣a)\>" ] , Print [ "\<Location:␣OUTSIDE␣the␣well␣(|x|␣>␣a)\>
   " ] ] , Print [ "\<No␣real␣interior␣nodes␣(x^2␣<␣0)\>" ] ] Print [ "
   \<\>" ] \
Print [ "\<Interpretation␣of␣Stationary␣Energy␣Value\>" ] Print [ "\<\>" ]
    \
Print [ ] Print [ "\<At␣the␣stationary␣point␣(d<E>/dr␣=␣0):\>" ] Print [ "
   \<\>" ] Print [ ] Print [ ] Print [ ] Print [ "\<\>" ] \
Print [ "\<Physical␣significance:\>" ] Print [ ] Print [ ] Print [ ] Print
    [ ] Print [ ] Print [ ] Print [ "\<\>" ] \
Print [ Framed [ Column [ { Style [ "\<ANSWER␣(Part␣e):\>" , , 14 ] ,
   Style [ , , 12 ] , Style [ , , 12 ] } ] , FrameStyle -> Thick ,
   Background -> LightYellow ] ] Print [ "\<\>" ] \
In[2285]:= a06db487-bbcc-ab40-b5ac-91c18f68f49b
```

INFINITE SQUARE WELL VARIATIONAL CALCULATION

Potential: V = 0 for -a ¡ x ¡ a, V = $\infty elsewhere$Boundary conditions: $\psi(\pm a) = 0$

PART (a): TRAPEZOIDAL TRIAL FUNCTION

Trial function:

$\psi(x) = a - |x| for b \leq |x| \leq a(slopedregions)$ $\psi(x) = a - b for |x| \leq b(flatregion)$

Case (i): b = 0 (Triangular function)

Normalization integral:

$N = \int_{-a}^{a}(a - |x|)^2 dx$ $Bysymmetry : N = 2\int_0^a (a-x)^2 dx$ $Expanding : \int_0^a (a^2 - 2ax + x^2)dx$ $= [a^2x - ax^2 + x^3/3]_0^a = a^3 - a^3 + a^3/3 = a^3/3$

A = $1/\sqrt{N}$ =

Kinetic energy calculation:

$d\psi/dx = -Afor0 < x < a$ $d\psi/dx = +Afor - a < x < 0 < T >= (\hbar^2/2m)\int_{-a}^{a} |d\psi/dx|^2 dx$ $= (\hbar^2/2m) \times 2\int_0^a A^2 dx = (\hbar^2/2m) \times 2A^2 a = (\hbar^2/2m)\times$

$< E >= (\hbar^2/2m) \times /a^2$ $ANSWER(Casei) :< E >= [formula]\hbar^2/(2ma^2)$

Case (ii): Optimize parameter b

Normalization integral:

$N = \int_{-a}^{a} \psi^2 dx = \int_{-a}^{-b}(a - |x|)^2 dx + \int_{-b}^{b}(a-b)^2 dx + \int_b^a (a - |x|)^2 dx$

By symmetry of outer regions:

$= 2\int_b^a (a-x)^2 dx + (a-b)^2(2b) = 2[(a-x)^3/(-3)]_b^a + 2b(a-b)^2 = 2(a-b)^3/3 + 2b(a-b)^2$

N(b) =

Kinetic energy calculation:

$d\psi/dx = 0for|x| < b(flatregioncontributesnothing)$ $d\psi/dx = -1forb < x < a$ $d\psi/dx = +1for - a < x < -b < T >= (\hbar^2/2m) \times 2\int_b^a (1/N)dx = (\hbar^2/2m) \times 2(a-b)/N = (\hbar^2/2m)\times$

Optimization:

$d < E > /db = (\hbar^2/2m)\times$ Since d¡E¿/db ¡ 0 for 0 ¡ b ¡ a, the energy decreases monotonically. Therefore, the minimum occurs at b = 0 (triangular function).

ANSWER (Case ii): Optimal value b = 0 (triangular function gives minimum)

PART (b): PARABOLIC TRIAL FUNCTION

$Trialfunction : \psi(x) = A(x-a)(x+a) = A(x^2 - a^2)$

Normalization integral:

$N = \int_{-a}^{a}(x^2 - a^2)^2 dx = \int_{-a}^{a}(x^4 - 2a^2x^2 + a^4)dx$

By symmetry (all terms are even):

$= 2\int_0^a (x^4 - 2a^2x^2 + a^4)dx = 2[x^5/5 - 2a^2x^3/3 + a^4x]_0^a = 2(a^5/5 - 2a^5/3 + a^5) = 2a^5(1/5 - 2/3 + 1)$ $= 2a^5(3/15 - 10/15 + 15/15) = 2a^5(8/15)$

$Derivative : d\psi/dx = 2Ax$

Kinetic energy calculation:

$< T >= (\hbar^2/2m)\int_{-a}^{a} |d\psi/dx|^2 dx = (\hbar^2/2m)\int_{-a}^{a}(2Ax)^2 dx = (\hbar^2/2m) \times 4A^2 \int_{-a}^{a} x^2 dx$

By symmetry:

$= (\hbar^2/2m) \times 4A^2 \times 2 \int_0^a x^2 dx = (\hbar^2/2m) \times 8A^2[x^3/3]_0^a = (\hbar^2/2m) \times 8A^2a^3/3 = (\hbar^2/2m) \times < E >=$
$(\hbar^2/2m) \times /a^2 \ ANSWER(Partb) :< E >= [formula]\hbar^2/(2ma^2)$

PART (c): QUARTIC TRIAL FUNCTION

$Trialfunction : \psi(x) = (a^2 - x^2)(\alpha x^2 + \beta) \ Variationalparameter : r = \alpha/\beta \ Expanding : \psi(x) =$
$(a^2 - x^2)(\alpha x^2 + \beta) = \alpha a^2 x^2 + \beta a^2 - \alpha x^4 - \beta x^2$

Normalization integral:

$N = \int_{-a}^{a}[(a^2-x^2)(\alpha x^2+\beta)]^2 dx = \int_{-a}^{a}[(\alpha a^2x^2+\beta a^2)^2 - 2(\alpha a^2x^2+\beta a^2)(\alpha x^4+\beta x^2)+(\alpha x^4+\beta x^2)^2]dx$

(All terms are even functions, so we integrate over symmetric limits)

Derivative calculation:

$d\psi/dx = d/dx[(a^2 - x^2)(\alpha x^2 + \beta)] \ Usingproductrule := (a^2 - x^2)(2\alpha x) + (\alpha x^2 + \beta)(-2x) =$
$2\alpha x(a^2 - x^2) - 2x(\alpha x^2 + \beta) = 2\alpha a^2 x - 2\alpha x^3 - 2\alpha x^3 - 2\beta x = 2\alpha a^2 x - 4\alpha x^3 - 2\beta x \ d\psi/dx =$

Kinetic energy integral:

$< T >= (\hbar^2/2m) \int_{-a}^{a} |d\psi/dx|^2 dx/N = (\hbar^2/2m) \int_{-a}^{a} (2\alpha a^2 x - 4\alpha x^3 - 2\beta x)^2 dx/N$

(Even function integrated over symmetric limits)

Numerator =

$< T >= (\hbar^2/2m) \times \ Energyasfunctionofr = \alpha/\beta : < E > (r) = (\hbar^2/2m) \times$

Variational condition d¡E¿/dr = 0:

$d < E > /dr = (\hbar^2/2m) \times$ Solutions for optimal r: $r_1 = r_2 =$

Energy values:

$Atr_1 :< E >= (\hbar^2/2m) \times /a^2 \ Atr_2 :< E >= (\hbar^2/2m) \times /a^2 \ Selectingr_2(minimumenergy)$

Optimal parameters:

$r_{opt} = < E >= (\hbar^2/2m) \times /a^2$

ANSWER (Part c):
Optimal r = formula]
$< E >= formula]\hbar^2/(2ma^2)$

PART (d): COMPARISON WITH EXACT RESULT

Exact ground state:

$\psi_0(x) = (1/\sqrt{a})cos(\pi x/(2a)) \ E_0 = \pi^2\hbar^2/(8ma^2) = (\hbar^2/2m) \times$

Summary of Variational Estimates

$Method < E > inunitsof(\hbar^2/2m)/a^2$

Exact

Triangular

Parabolic

Quartic (optimized)

$Verification: All variational estimates satisfy < E >\geq E_0$ $Triangular :\geq$ ✓ $Parabolic :\geq$ ✓ $Quartic :\geq$ ✓

ANSWER (Part d):
$All variational estimates satisfy < E >\geq E_0$
The quartic trial function gives the best approximation.

Mean-Square Deviations

$Formula: \Delta^2 = \int |\psi_0 - \psi_t|^2 dx = 2(1 - \int \psi_0 \psi_t dx) for normalized functions$

Parabolic function:

$Overlap: \int_{-a}^{a} \psi_0 \psi_t dx = Mean-square deviation: \Delta^2 = Interpretation: Smaller \Delta^2 indicates better approximatio$
PART (e): NODES OF OPTIMAL QUARTIC AND INTERPRETATION $Optimized quartic:$
$\psi(x) = A(a^2 - x^2)(\alpha x^2 + \beta) with r = \alpha/\beta =$

Nodes occur at:

$(1) Boundary: x = \pm a (required by boundary conditions)$ $(2) Interior: where \alpha x^2 + \beta = 0, i.e., x^2 = -\beta/\alpha = -1/r$ $Interior node condition: x^2 = -1/r = Real interior nodes exist at x^2 = Location:$
$INSIDE the well (|x| < a) Location: OUTSIDE the well (|x| > a) No real interior nodes (x^2 < 0)$

Interpretation of Stationary Energy Value

The variational method minimizes ¡E¿ within the family of quartic trial functions. At the stationary point (d¡E¿/dr = 0): •$The energy is minimized with respect to the parameter r$ •$This provides an upper bound :< E >\geq E_0 (variational theorem)$ •$The optimal function best approximates the true ground state within this family$

Physical significance:

•$The optimization balances kinetic energy (prefers smoothness) with boundary conditions (requires \psi(\pm a) = 0)$ •$The true ground state cos(\pi x/2a) has NO interior nodes$ •$Our quartic approximation may have nodes depending on$
•$The stationary condition d < E > /dr = 0 is the variational analog of the Schrödinger equation, ensuring the functi$

ANSWER (Part e):
$The stationary energy represents the best approximation to E_0$
$within the chosen family, guaranteed to be \geq E_0.$

Input:

```
ClearAll [ "\<Global`*\>" ] \
(* Set parameters *) \
a = 1 ; (* length parameter *) g = 1 ; (* potential strength , in units of
    [HBar]\.b2 / ( ma ) *) \
Print [ Style [ "\<Linear␣Potential␣V(x)␣=␣g|x|␣-␣Rayleigh-Ritz␣Method\>"
   , , 16 ] ] \
\
(* === === === = STEP 1 : Define Basis Functions === === === = *) Print [
   Style [ "\<STEP␣1:␣Basis␣Functions\>" , , 14 ] ] f1 [ x_ ] := Exp [ - x
    ^ 2 / a ^ 2 ] f2 [ x_ ] := x * Exp [ - x ^ 2 / a ^ 2 ] \
Print [ "\<f\:2081(x)␣=␣exp(-x\.b2/a\.b2)␣[EVEN␣function]\>" ] Print [ "\<
   f\:2082(x)␣=␣x[CenterDot]exp(-x\.b2/a\.b2)␣[ODD␣function]\>" ] Print [
   ] \
(* Plot basis functions - BLACK AND WHITE *) \
Plot [ { f1 [ x ] , f2 [ x ] } , { x , - 3 , 3 } , PlotStyle -> { { Black
   , Thick } , (* f1 : solid black *) { Black , Dashed , Thick } (* f2 :
   dashed black *) } , PlotLegends -> Placed [ LineLegend [ { Graphics [ {
    Black , Thick , Line [ { { 0 , 0 } , { 1 , 0 } } ] } ] , Graphics [ {
   Black , Dashed , Thick , Line [ { { 0 , 0 } , { 1 , 0 } } ] } ] } , { "
   \<f\:2081(x)␣[solid]\>" , "\<f\:2082(x)␣[dashed]\>" } ] , { Right , Top
    } ] , PlotLabel -> Style [ "\<Basis␣Functions\>" , ] , AxesLabel -> {
   Style [ "\<x\>" , 12 ] , Style [ "\<f(x)\>" , 12 ] } , GridLines ->
   Automatic , GridLinesStyle -> Directive [ Gray , Dotted ] , ImageSize
   -> Large , Frame -> True , FrameStyle -> Black ] \
(* === === === = STEP 2 : Overlap Matrix S === === === = *) \
Print [ Style [ , , 14 ] ] Print [ ] \
S11 = Integrate [ f1 [ x ] ^ 2 , { x , - Infinity , Infinity } ,
   Assumptions -> a > 0 ] Print [ "\<S\:2081\:2081␣=␣[Integral]␣f\:2081\.
   b2␣dx␣=␣\>" , S11 ] Print [ "\<␣=␣\>" , N [ S11 , 6 ] ] Print [ ] \
S12 = Integrate [ f1 [ x ] * f2 [ x ] , { x , - Infinity , Infinity } ,
   Assumptions -> a > 0 ] Print [ , S12 , "\<␣(odd␣integrand␣[RightArrow]␣
   0)\>" ] Print [ ] \
S21 = S12 ; Print [ "\<S\:2082\:2081␣=␣S\:2081\:2082␣=␣\>" , S21 ] Print [
    ] \
S22 = Integrate [ f2 [ x ] ^ 2 , { x , - Infinity , Infinity } ,
   Assumptions -> a > 0 ] Print [ "\<S\:2082\:2082␣=␣[Integral]␣f\:2082\.
   b2␣dx␣=␣\>" , S22 ] Print [ "\<␣=␣\>" , N [ S22 , 6 ] ] Print [ ] \
(* Construct overlap matrix *) \
Smatrix = { { S11 , S12 } , { S21 , S22 } } ; Print [ "\<Overlap␣Matrix␣S␣
   (symbolic):\>" ] Print [ MatrixForm [ Smatrix ] ] Print [ ] Print [ "\<
   Overlap␣Matrix␣S␣(numerical):\>" ] Print [ MatrixForm [ N [ Smatrix , 6
    ] ] ] Print [ ] \
(* === === === = STEP 3 : Kinetic Energy Matrix T === === === = *) \
Print [ Style [ , , 14 ] ] Print [ ] \
(* Calculate second derivatives *) \
f1pp [ x_ ] = D [ f1 [ x ] , { x , 2 } ] f2pp [ x_ ] = D [ f2 [ x ] , { x
   , 2 } ] \
Print [ "\<d\.b2f\:2081/dx\.b2␣=␣\>" , f1pp [ x ] ] Print [ ] Print [ "\<d
   \.b2f\:2082/dx\.b2␣=␣\>" , f2pp [ x ] ] Print [ ] \
```

```
T11 = - 1 / 2 * Integrate [ f1 [ x ] * f1pp [ x ] , { x , - Infinity ,
    Infinity } , Assumptions -> a > 0 ] Print [ , T11 ] Print [ "\<␣=␣\>" ,
     N [ T11 , 6 ] ] Print [ ] \
T12 = - 1 / 2 * Integrate [ f1 [ x ] * f2pp [ x ] , { x , - Infinity ,
    Infinity } , Assumptions -> a > 0 ] Print [ , T12 , "\<␣(parity␣[
    RightArrow]␣0)\>" ] Print [ ] \
T21 = T12 ; Print [ "\<T\:2082\:2081␣=␣T\:2081\:2082␣=␣\>" , T21 ] Print [
     ] \
T22 = - 1 / 2 * Integrate [ f2 [ x ] * f2pp [ x ] , { x , - Infinity ,
    Infinity } , Assumptions -> a > 0 ] Print [ , T22 ] Print [ "\<␣=␣\>" ,
     N [ T22 , 6 ] ] Print [ ] \
(* Construct kinetic energy matrix *) \
Tmatrix = { { T11 , T12 } , { T21 , T22 } } ; Print [ "\<Kinetic␣Energy␣
    Matrix␣T␣(symbolic):\>" ] Print [ MatrixForm [ Tmatrix ] ] Print [ ]
    Print [ "\<Kinetic␣Energy␣Matrix␣T␣(numerical):\>" ] Print [ MatrixForm
     [ N [ Tmatrix , 6 ] ] ] Print [ ] \
(* === === === = STEP 4 : Potential Energy Matrix V === === === = *) \
Print [ Style [ , , 14 ] ] Print [ ] \
V11 = g * Integrate [ Abs [ x ] * f1 [ x ] ^ 2 , { x , - Infinity ,
    Infinity } , Assumptions -> a > 0 ] Print [ , V11 ] Print [ "\<␣=␣\>" ,
     N [ V11 , 6 ] ] Print [ ] \
V12 = g * Integrate [ Abs [ x ] * f1 [ x ] * f2 [ x ] , { x , - Infinity ,
     Infinity } , Assumptions -> a > 0 ] Print [ , V12 , "\<␣(parity␣[
    RightArrow]␣0)\>" ] Print [ ] \
V21 = V12 ; Print [ "\<V\:2082\:2081␣=␣V\:2081\:2082␣=␣\>" , V21 ] Print [
     ] \
V22 = g * Integrate [ Abs [ x ] * f2 [ x ] ^ 2 , { x , - Infinity ,
    Infinity } , Assumptions -> a > 0 ] Print [ , V22 ] Print [ "\<␣=␣\>" ,
     N [ V22 , 6 ] ] Print [ ] \
(* Construct potential energy matrix *) \
Vmatrix = { { V11 , V12 } , { V21 , V22 } } ; Print [ "\<Potential␣Energy␣
    Matrix␣V␣(symbolic):\>" ] Print [ MatrixForm [ Vmatrix ] ] Print [ ]
    Print [ "\<Potential␣Energy␣Matrix␣V␣(numerical):\>" ] Print [
    MatrixForm [ N [ Vmatrix , 6 ] ] ] Print [ ] \
(* === === === = STEP 5 : Hamiltonian Matrix H = T + V === === === = *) \
Print [ Style [ "\<STEP␣5:␣Hamiltonian␣Matrix␣H␣=␣T␣+␣V\>" , , 14 ] ]
    Print [ ] \
Hmatrix = Tmatrix + Vmatrix ; Print [ "\<Hamiltonian␣Matrix␣H␣(symbolic)
    :\>" ] Print [ MatrixForm [ Simplify [ Hmatrix ] ] ] Print [ ] Print [
    "\<Hamiltonian␣Matrix␣H␣(numerical):\>" ] Print [ MatrixForm [ N [
    Hmatrix , 6 ] ] ] Print [ ] \
Print [ Style [ "\<***␣KEY␣OBSERVATION:␣H␣and␣S␣are␣BLOCK-DIAGONAL!␣***\>"
     , ] ] Print [ "\<All␣off-diagonal␣elements␣are␣ZERO␣due␣to␣parity␣
    symmetry.\>" ] Print [ "\<Even␣function␣f\:2081␣doesn't␣mix␣with␣odd␣
    function␣f\:2082.\>" ] Print [ ] \
(* === === === = STEP 6 : Solve Generalized Eigenvalue Problem === === ===
     = *) \
Print [ Style [ "\<STEP␣6:␣Solve␣HC␣=␣SCE\>" , , 14 ] ] Print [ ] \
(* Numerical solution *) \
{ evalues , evectors } = Eigensystem [ { N [ Hmatrix ] , N [ Smatrix ] } ]
     ; sortedIndices = Ordering [ evalues ] ; evalues = evalues [ [
    sortedIndices ] ] ; evectors = evectors [ [ sortedIndices ] ] ; \
Print [ "\<Rayleigh-Ritz␣Energy␣Eigenvalues:\>" ] Print [ "\<E\:2081␣=␣\>"
     , NumberForm [ evalues [ [ 1 ] ] , 6 ] ] Print [ "\<E\:2082␣=␣\>" ,
```

```
    NumberForm [ evalues [ [ 2 ] ] , 6 ] ] Print [ ] \
Print [ "\<Eigenvectors␣(coefficients␣[c\:2081,␣c\:2082]):\>" ] Print [ "
    \<Ground␣state:␣c␣=␣[\>" , NumberForm [ evectors [ [ 1 , 1 ] ] , 4 ] ,
    "\<,␣\>" , NumberForm [ evectors [ [ 1 , 2 ] ] , 4 ] , "\<]\>" ] Print
    [ "\<Excited␣state:␣c␣=␣[\>" , NumberForm [ evectors [ [ 2 , 1 ] ] , 4
    ] , "\<,␣\>" , NumberForm [ evectors [ [ 2 , 2 ] ] , 4 ] , "\<]\>" ]
    Print [ ] \
(* === === === = STEP 7 : Analytical Formulas === === === = *) \
Print [ Style [ "\<STEP␣7:␣Analytical␣Energy␣Formulas␣(Block-Diagonal)\>"
    , , 14 ] ] Print [ ] \
Print [ "\<Since␣H␣and␣S␣are␣block-diagonal,␣eigenvalues␣are:\>" ] Print [
     ] E1analytical = Hmatrix [ [ 1 , 1 ] ] / Smatrix [ [ 1 , 1 ] ] ;
    E2analytical = Hmatrix [ [ 2 , 2 ] ] / Smatrix [ [ 2 , 2 ] ] ; \
Print [ "\<E\:2081␣=␣H\:2081\:2081/S\:2081\:2081␣=␣\>" , Simplify [
    E1analytical ] ] Print [ "\<␣=␣\>" , N [ E1analytical , 6 ] ] Print [ ]
     Print [ "\<E\:2082␣=␣H\:2082\:2082/S\:2082\:2082␣=␣\>" , Simplify [
    E2analytical ] ] Print [ "\<␣=␣\>" , N [ E2analytical , 6 ] ] Print [ ]
     \
(* === === === = STEP 8 : Compare with Exact Results === === === = *) \
Print [ Style [ "\<STEP␣8:␣Comparison␣with␣Exact␣(Analytic)␣Results\>" , ,
     14 ] ] Print [ ] \
Print [ "\<For␣the␣linear␣potential␣V(x)␣=␣g|x|,␣the␣exact␣solution\>" ]
    Print [ "\<involves␣Airy␣functions.␣The␣energy␣eigenvalues␣are:\>" ]
    Print [ ] Print [ "\<␣E\:2099␣=␣g^(2/3)␣[CenterDot]␣|[Alpha]\:2099|\>"
    ] Print [ ] Print [ ] Print [ ] \
(* Zeros of Airy function Ai ( - z ) - these are negative of the usual
    zeros *) \
airyZeros = { 2.33810741 , 4.08794944 , 5.52055983 } ; \
(* For g = 1 , the exact energies are *) \
exactE1 = g ^ ( 2 / 3 ) * airyZeros [ [ 1 ] ] ; exactE2 = g ^ ( 2 / 3 ) *
    airyZeros [ [ 2 ] ] ; exactE3 = g ^ ( 2 / 3 ) * airyZeros [ [ 3 ] ] ; \
Print [ "\<Exact␣energy␣levels␣(from␣Airy␣function):\>" ] Print [ "\<E
    \:2081(exact)␣=␣\>" , NumberForm [ exactE1 , 6 ] ] Print [ "\<E\:2082(
    exact)␣=␣\>" , NumberForm [ exactE2 , 6 ] ] Print [ "\<E\:2083(exact)␣=
    ␣\>" , NumberForm [ exactE3 , 6 ] ] Print [ ] \
Print [ Style [ "\<COMPARISON␣TABLE:\>" , , 12 ] ] Print [ StringRepeat [
    "\<-\>" , 72 ] ] Print [ Style [ StringForm [ "\<‘‘␣‘‘␣‘‘␣‘‘\>" ,
    StringPadRight [ "\<Level\>" , 8 ] , StringPadRight [ "\<Rayleigh-Ritz
    \>" , 16 ] , StringPadRight [ "\<Exact\>" , 16 ] , "\<Error␣(%)\>" ] ,
    ] ] Print [ StringRepeat [ "\<-\>" , 72 ] ] \
err1 = 100 * Abs [ evalues [ [ 1 ] ] - exactE1 ] / exactE1 ; err2 = 100 *
    Abs [ evalues [ [ 2 ] ] - exactE2 ] / exactE2 ; \
Print [ StringForm [ "\<‘‘␣‘‘␣‘‘␣‘‘\>" , StringPadRight [ "\<E\:2081\>" ,
    8 ] , StringPadRight [ ToString [ NumberForm [ evalues [ [ 1 ] ] , 6 ]
    ] , 16 ] , StringPadRight [ ToString [ NumberForm [ exactE1 , 6 ] ] ,
    16 ] , NumberForm [ err1 , { 5 , 2 } ] ] ] \
Print [ StringForm [ "\<‘‘␣‘‘␣‘‘␣‘‘\>" , StringPadRight [ "\<E\:2082\>" ,
    8 ] , StringPadRight [ ToString [ NumberForm [ evalues [ [ 2 ] ] , 6 ]
    ] , 16 ] , StringPadRight [ ToString [ NumberForm [ exactE2 , 6 ] ] ,
    16 ] , NumberForm [ err2 , { 5 , 2 } ] ] ] \
Print [ StringRepeat [ "\<-\>" , 72 ] ] Print [ ] \
(* === === === = STEP 9 : Visualization === === === = *) \
Print [ Style [ "\<STEP␣9:␣Visualization␣of␣Results\>" , , 14 ] ] Print [
    ] \
```

```
(* Construct approximate wavefunctions *) \
psi1 [ x_ ] := evectors [ [ 1 , 1 ] ] * f1 [ x ] + evectors [ [ 1 , 2 ] ]
   * f2 [ x ] psi2 [ x_ ] := evectors [ [ 2 , 1 ] ] * f1 [ x ] + evectors
   [ [ 2 , 2 ] ] * f2 [ x ] \
(* Normalize *) \
norm1 = Sqrt [ NIntegrate [ psi1 [ x ] ^ 2 , { x , - 5 , 5 } ] ] ; norm2 =
    Sqrt [ NIntegrate [ psi2 [ x ] ^ 2 , { x , - 5 , 5 } ] ] ; psi1n [ x_
   ] := psi1 [ x ] / norm1 psi2n [ x_ ] := psi2 [ x ] / norm2 \
(* Plot wavefunctions - BLACK AND WHITE *) \
Plot [ { psi1n [ x ] , psi2n [ x ] } , { x , - 3 , 3 } , PlotStyle -> { {
   Black , Thick } , (* [Psi]1 : solid *) { Black , Dashed , Thick } (* [
   Psi]2 : dashed *) } , PlotLegends -> Placed [ LineLegend [ { Graphics [
    { Black , Thick , Line [ { { 0 , 0 } , { 1 , 0 } } ] } ] , Graphics [
   { Black , Dashed , Thick , Line [ { { 0 , 0 } , { 1 , 0 } } ] } ] } , {
    "\<[Psi]\:2081(x)␣Ground␣[solid]\>" , "\<[Psi]\:2082(x)␣Excited␣[
   dashed]\>" } ] , { Right , Top } ] , PlotLabel -> Style [ "\<
   Approximate␣Wavefunctions␣(Rayleigh-Ritz)\>" , ] , AxesLabel -> { Style
    [ "\<x\>" , 12 ] , Style [ "\<[Psi](x)\>" , 12 ] } , GridLines ->
   Automatic , GridLinesStyle -> Directive [ Gray , Dotted ] , ImageSize
   -> Large , Frame -> True , FrameStyle -> Black ] \
(* Plot potential and energy levels - BLACK AND WHITE *) \
Show [ (* Potential *) Plot [ g * Abs [ x ] , { x , - 3 , 3 } , PlotStyle
   -> { Black , Thick } , PlotRange -> { 0 , 5 } ] , (* Rayleigh - Ritz E1
    *) Graphics [ { Black , Thick , Line [ { { - 3 , evalues [ [ 1 ] ] } ,
    { 3 , evalues [ [ 1 ] ] } } ] , Text [ Style [ "\<E\:2081(RR)=\>" <>
   ToString [ NumberForm [ evalues [ [ 1 ] ] , 3 ] ] , 11 , ] , { - 2.3 ,
   evalues [ [ 1 ] ] + 0.25 } ] } ] , (* Rayleigh - Ritz E2 *) Graphics [
   { Black , Thick , Line [ { { - 3 , evalues [ [ 2 ] ] } , { 3 , evalues
   [ [ 2 ] ] } } ] , Text [ Style [ "\<E\:2082(RR)=\>" <> ToString [
   NumberForm [ evalues [ [ 2 ] ] , 3 ] ] , 11 , ] , { - 2.3 , evalues [ [
    2 ] ] + 0.25 } ] } ] , (* Exact E1 *) Graphics [ { Black , Dashed ,
   Line [ { { - 3 , exactE1 } , { 3 , exactE1 } } ] , Text [ Style [ "\<E
   \:2081(exact)=\>" <> ToString [ NumberForm [ exactE1 , 3 ] ] , 10 ] , {
    2.0 , exactE1 - 0.25 } ] } ] , (* Exact E2 *) Graphics [ { Black ,
   Dashed , Line [ { { - 3 , exactE2 } , { 3 , exactE2 } } ] , Text [
   Style [ "\<E\:2082(exact)=\>" <> ToString [ NumberForm [ exactE2 , 3 ]
   ] , 10 ] , { 2.0 , exactE2 - 0.25 } ] } ] , PlotLabel -> Style [ "\<
   Linear␣Potential␣V(x)=g|x|␣with␣Energy␣Levels\>" , , 13 ] , AxesLabel
   -> { Style [ "\<x\>" , 12 ] , Style [ "\<Energy\>" , 12 ] } , ImageSize
    -> Large , Frame -> True , FrameStyle -> Black , GridLines ->
   Automatic , GridLinesStyle -> Directive [ Gray , Dotted ] , (* Legend
   *) Epilog -> { Text [ Style [ "\<Solid␣lines:␣Rayleigh-Ritz\>" , 10 ] ,
    { - 2.2 , 4.5 } ] , Text [ Style [ "\<Dashed␣lines:␣Exact\>" , 10 ] ,
   { - 2.2 , 4.2 } ] , Text [ Style [ "\<Thick␣line:␣Potential␣V(x)\>" ,
   10 ] , { - 2.2 , 3.9 } ] } ] \
(* === === === = STEP 10 : Comments and Analysis === === === = *) \
Print [ Style [ "\<STEP␣10:␣Analysis␣and␣Comments\>" , , 14 ] ] Print [ ]
   \
Print [ "\<1.␣PARITY␣SYMMETRY:\>" ] Print [ "\<␣[Bullet]␣V(x)␣=␣g|x|␣is␣
   EVEN:␣V(-x)␣=␣V(x)\>" ] Print [ "\<␣[Bullet]␣f\:2081(x)␣is␣EVEN:␣f
   \:2081(-x)␣=␣f\:2081(x)\>" ] Print [ "\<␣[Bullet]␣f\:2082(x)␣is␣ODD:␣f
   \:2082(-x)␣=␣-f\:2082(x)\>" ] Print [ ] Print [ ] \
Print [ "\<2.␣BLOCK-DIAGONAL␣STRUCTURE:\>" ] Print [ "\<␣[Bullet]␣
   Hamiltonian␣separates␣into␣even␣and␣odd␣sectors\>" ] Print [ ] Print [
```

```
    ] Print [ ] \
Print [ "\<3. ACCURACY OF RAYLEIGH-RITZ:\>" ] Print [ "\< [Bullet] Ground
    state error: \>" , NumberForm [ err1 , { 5 , 2 } ] , "\<%\>" ] Print [
    "\< [Bullet] Excited state error: \>" , NumberForm [ err2 , { 5 , 2 } ]
     , "\<%\>" ] Print [ "\< [Bullet] Excellent for only 2 basis functions
    !\>" ] Print [ "\< [Bullet] RR method provides UPPER BOUNDS to true
    energies\>" ] Print [ ] \
Print [ "\<4. VARIATIONAL PRINCIPLE VERIFICATION:\>" ] Print [ "\< [Bullet
    ] E\:2081(RR) [GreaterEqual] E\:2081(exact)? \>" , evalues [ [ 1 ] ] >=
     exactE1 ] Print [ "\< [Bullet] E\:2082(RR) [GreaterEqual] E\:2082(
    exact)? \>" , evalues [ [ 2 ] ] >= exactE2 ] Print [ ] Print [ ] \
Print [ "\<5. PHYSICAL INTERPRETATION:\>" ] Print [ "\< [Bullet] Linear
    potential g|x| is a 'V-shaped' well\>" ] Print [ ] Print [ "\< [Bullet]
    Ground state: concentrated near x=0, no nodes\>" ] Print [ "\< [
    Bullet] Excited state: has node at x=0 (odd parity)\>" ] Print [ ] \
Print [ "\<6. WHY THE METHOD WORKS WELL:\>" ] Print [ "\< [Bullet]
    Gaussian basis captures the localized nature\>" ] Print [ "\< [Bullet]
    Parity structure exactly preserved\>" ] Print [ "\< [Bullet]
    Variational freedom via linear combinations\>" ] Print [ ] \
In[4731]:= db1085e3-a732-bc42-ba4f-77b237bb4e4d
```

Linear Potential V(x) = g—x— - Rayleigh-Ritz Method

STEP 1: Basis Functions

$f\,2081(x) = exp(-x^2/a^2)[EVENfunction]$ $f\,2082(x) = xCenterDot]exp(-x^2/a^2)[ODDfunction]$

Figure placeholder: Export figure$_1$*.pngfromMathematicaspace*1*cm*

Figure 1: Figure 1

STEP 2: Overlap Matrix Elements S 1d62 2c7c = 27e8f 1d62—f 2c7c 27e9

$S20812081 = \int f2081^2 dx =$ S 2081 2082 $= \int f2081CenterDot]f2082dx =$ "","","0","","" $(oddintegrand \to 0)$

S 2082 2081 = S 2081 2082 =

S 2082 2082 $= \int f$ $2082^2 dx =$

Overlap Matrix S (symbolic):

Overlap Matrix S (numerical):

$STEP3 : KineticEnergyMatrixT$ 1d62 2c7c $= -\dot{b}d$ 27e8f 1d62$|d^2/dx^2|f$ 2c7c 27e9 $d^2 f$ $2081/dx^2 =$ $d^2 f$ $2082/dx^2 =$

T 2081 2081 = -$\dot{\mathbf{b}}$d$\int f$ $2081CenterDot]f$ $2081''dx =$

T 2081 2082 = -$\dot{\mathbf{b}}$d$\int f$ $2081CenterDot]f$ $2082''dx = (parity \to 0)$

T 2082 2081 = T 2081 2082 =

T 2082 2082 = -ḃd$\int f\,2082CenterDot]f\,2082''dx =$

Kinetic Energy Matrix T (symbolic):

Kinetic Energy Matrix T (numerical):

STEP 4: Potential Energy Matrix V 1d62 2c7c = g 27e8f 1d62——x——f 2c7c 27e9
$V20812081 = g\int |x|CenterDot]f2081^2dx =$ **V 2081 2082 = g**$\int |x|CenterDot]f2081CenterDot]f2082dx =$
$(parity \to 0)$

V 2082 2081 = V 2081 2082 =

$V\,2082\,2082 = g\int |x|CenterDot]f\,2082^2dx =$

Potential Energy Matrix V (symbolic):

Potential Energy Matrix V (numerical):

STEP 5: Hamiltonian Matrix H = T + V

Hamiltonian Matrix H (symbolic):

Hamiltonian Matrix H (numerical):

***** KEY OBSERVATION: H and S are BLOCK-DIAGONAL! *****

All off-diagonal elements are ZERO due to parity symmetry.

Even function f 2081 doesn't mix with odd function f 2082.

STEP 6: Solve HC = SCE

Rayleigh-Ritz Energy Eigenvalues:

E 2081 = 0.898942

E 2082 = 2.29788

Eigenvectors (coefficients [c 2081, c 2082]):

Ground state: c = [1. , 0.]

Excited state: c = [0. , 1.]

STEP 7: Analytical Energy Formulas (Block-Diagonal) Since H and S are block-diagonal, eigenvalues are:

E 2081 = H 2081 2081/S 2081 2081 =

E 2082 = H 2082 2082/S 2082 2082 =

STEP 8: Comparison with Exact (Analytic) Results For the linear potential V(x) = g—x—, the exact solution involves Airy functions. The energy eigenvalues are:
$E\,2099 = g^(2/3)CenterDot]|\alpha\,2099|\ where\alpha\,2099arethezerosoftheAiryfunctionAi(-z).$

Exact energy levels (from Airy function):

E 2081(exact) = 2.33811
E 2082(exact) = 4.08795
E 2083(exact) = 5.52056
COMPARISON TABLE:

E 2081 0.898942 2.33811 $RowBox[\ddot{6}1.55\ddot{]}$

E 2082 2.29788 4.08795 $RowBox[\ddot{4}3.79\ddot{]}$

STEP 9: Visualization of Results

Figure placeholder: Export figure$_2$*.png from Mathematica space* 1*cm*

Figure 2: Figure 2

Figure placeholder: Export figure$_3$*.png from Mathematica space* 1*cm*

Figure 3: Figure 3

STEP 10: Analysis and Comments

1. PARITY SYMMETRY:

$\bullet V(x) = g|x|isEVEN : V(-x) = V(x)$ $\bullet$ $27e8f\ 2081|O|f\ 2082\ 27e9 = 0 for any even operator O$

2. BLOCK-DIAGONAL STRUCTURE:

$\bullet Hamiltonian separates into even and odd sectors$ $\bullet Ground state : EVEN parity(only f 2081, c2081 \neq 0, c\,2082 = 0)$ $\bullet First excited : ODD parity(only f\ 2082, c\,2081 = 0, c\,2082 \neq 0)$

3. ACCURACY OF RAYLEIGH-RITZ:

$\bullet Ground state error : 61.5543.79$

4. VARIATIONAL PRINCIPLE VERIFICATION:

$\bullet E2081(RR) \geq E2081(exact)?$ $\bullet E2082(RR) \geq E2082(exact)?$ $\bullet Approximate energies are indeed upper bounds \checkmark$

5. PHYSICAL INTERPRETATION:

$\bullet Linear potential g|x| is a 'V-shaped' well \bullet With g = \hbar^2/(ma) = 1, length scale set by a = 1 \bullet Ground state : concentrated near x = 0, no nodes \bullet Excited state : has node at x = 0 (odd parity)$ **6. WHY THE METHOD WORKS WELL:** $\bullet Parity structure exactly preserved$

$\bullet Variational freedom via linear combinations$

HW 8-1 pb 8 November 3, 2025

Input:

```
(* Barrier in a Well - Variational Method *) (* Natural units : [HBar] = m
    = a = 1 *) (* Parameters : [Sigma] = 1 / 10 , V\:2080 = 4 *) \
a = 1 ; [Sigma] = 1 / 10 ; V0 = 4 ; \
(* Basis functions and potential *) \
[Psi] [ n_Integer , x_ ? NumericQ ] := Sqrt [ 2 ] Sin [ n [Pi] x ] V [ x_
   ? NumericQ ] := V0 Exp [ - ( x - 1 / 2 ) ^ 2 / ( 2 [Sigma] ^ 2 ) ] \
(* Matrix elements *) \
T [ i_ , j_ ] := If [ i == j , ( [Pi] ^ 2 i ^ 2 ) / 2 , 0 ] \
Vmatrix [ i_ , j_ ] := NIntegrate [ [Psi] [ i , x ] V [ x ] [Psi] [ j , x
   ] , { x , 0 , 1 } , Method -> { "\<GlobalAdaptive\>" , "\<
   MaxErrorIncreases\>" -> 10000 } , MinRecursion -> 3 , MaxRecursion ->
   20 , WorkingPrecision -> 16 ] \
(* Build Hamiltonian and find lowest 4 energies *) \
FindEnergies [ n_ ] := Module [ { H , result } , H = Table [ T [ i , j ] +
    Vmatrix [ i , j ] , { i , n } , { j , n } ] ; \
result = Sort [ Eigenvalues [ N [ H ] ] ] ; \
Return [ result [ [ 1 ;; 4 ] ] ] ] \
\
(* RESULTS *) \
Print [ Style [ "\<Lowest␣Four␣Energy␣Levels\>" , , 16 ] ] ; Print [ Style
    [ "\<(in␣natural␣units␣where␣[HBar]␣=␣m␣=␣a␣=␣1)\>" , , 12 ] ] ; Print
    [ ] ; \
(* Part ( a ) : n = 4 *) \
energies4 = FindEnergies [ 4 ] ; Print [ Style [ "\<(a)␣n␣=␣4␣basis␣
   functions\>" , , 14 ] ] ; Print [ Grid [ Prepend [ Table [ { "\<E\>" <>
    ToString [ i ] , NumberForm [ energies4 [ [ i ] ] , { 6 , 4 } ] } , {
   i , 1 , 4 } ] , { "\<Level\>" , "\<Energy\>" } ] , Frame -> All ,
   Background -> { None , { LightBlue , { White , LightGray } } } ,
   Alignment -> { { Left , Right } } , Spacings -> { 2 , 1 } ] ] ; \
(* Part ( b ) : n = 6 *) \
energies6 = FindEnergies [ 6 ] ; Print [ "\<\
\>" , Style [ "\<(b)␣n␣=␣6␣basis␣functions\>" , , 14 ] ] ; Print [ Grid [
   Prepend [ Table [ { "\<E\>" <> ToString [ i ] , NumberForm [ energies6
   [ [ i ] ] , { 6 , 4 } ] } , { i , 1 , 4 } ] , { "\<Level\>" , "\<Energy
   \>" } ] , Frame -> All , Background -> { None , { LightBlue , { White ,
    LightGray } } } , Alignment -> { { Left , Right } } , Spacings -> { 2
   , 1 } ] ] ; \
(* Part ( c ) : n = 8 *) \
energies8 = FindEnergies [ 8 ] ; Print [ "\<\
\>" , Style [ "\<(c)␣n␣=␣8␣basis␣functions\>" , , 14 ] ] ; Print [ Grid [
   Prepend [ Table [ { "\<E\>" <> ToString [ i ] , NumberForm [ energies8
   [ [ i ] ] , { 6 , 4 } ] } , { i , 1 , 4 } ] , { "\<Level\>" , "\<Energy
   \>" } ] , Frame -> All , Background -> { None , { LightBlue , { White ,
    LightGray } } } , Alignment -> { { Left , Right } } , Spacings -> { 2
   , 1 } ] ] ; \
(* Comparison table *) \
Print [ "\<\
\>" , Style [ "\<Comparison␣of␣Results\>" , , 14 ] ] ; Print [ Grid [
   Prepend [ Table [ { "\<E\>" <> ToString [ i ] , NumberForm [ energies4
   [ [ i ] ] , { 6 , 4 } ] , NumberForm [ energies6 [ [ i ] ] , { 6 , 4 }
```

```
] , NumberForm [ energies8 [ [ i ] ] , { 6 , 4 } ] } , { i , 1 , 4 } ]
, { "\<Level\>" , "\<n␣=␣4\>" , "\<n␣=␣6\>" , "\<n␣=␣8\>" } ] , Frame
-> All , Background -> { None , { LightBlue , { White , LightGray } } }
 , Alignment -> { { Left , Right , Right , Right } } , Spacings -> { 2
, 1 } ] ] ;
```

Lowest Four Energy Levels

$(in natural units where \hbar = m = a = 1)$ $Units : \hbar^2/(2ma^2) or equivalently \pi^2\hbar^2/(2ma^2) \times (n/\pi)^2$

(a) n = 4 basis functions

Level	Energy
E1	6.7185
E2	20.2795
E3	45.6276
E4	79.9240

(b) n = 6 basis functions

Level	Energy
E1	6.7154
E2	20.2784
E3	45.6176
E4	79.9172

(c) n = 8 basis functions

Level	Energy
E1	6.7153
E2	20.2783
E3	45.6166
E4	79.9164

Comparison of Results

Level	n = 4	n = 6	n = 8
E1	6.7185	6.7154	6.7153
E2	20.2795	20.2784	20.2783
E3	45.6276	45.6176	45.6166
E4	79.9240	79.9172	79.9164