

HW 8-1 pb 5-all

November 3, 2025

Input:

```
ClearAll [ "\<Global`*`" ] \
(* Set parameters *) \
a = 1 ; (* length parameter *) g = 1 ; (* potential strength , in units of
[HBar]\.b2 / ( ma ) *) \
Print [ Style [ "\<LinearPotential`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 *) \
```

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Smatrix = { { S11 , S12 } , { S21 , S22 } } ; Print [ "<\OverlapMatrixS
(symbolic):>" ] Print [ MatrixForm [ Smatrix ] ] Print [ ] Print [ "<\OverlapMatrixS(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 [ "(parityu[
RightArrow]u0)>" ] Print [ ] \
T21 = T12 ; Print [ "(parityu[
RightArrow]u0)>" ] Print [ ] \
V21 = V12 ; Print [ "

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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 *) \
{ evaluates , eigenvectors } = Eigensystem [ { N [ Hmatrix ] , N [ Smatrix ] } ]
; sortedIndices = Ordering [ evaluates ] ; evaluates = evaluates [ [ sortedIndices ] ] ; eigenvectors = eigenvectors [ [ sortedIndices ] ] ; \
Print [ "\<Rayleigh-Ritz Energy Eigenvalues:\>" ] Print [ "\<E\>:2081\>" ,
NumberForm [ evaluates [ [ 1 ] ] , 6 ] ] Print [ "\<E\>:2082\>" ,
NumberForm [ evaluates [ [ 2 ] ] , 6 ] ] Print [ ] \
Print [ "\<Eigenvectors(coefficients[c\>:2081,c\>:2082]):\>" ] Print [ "
\<Ground state:c\>" , NumberForm [ eigenvectors [ [ 1 , 1 ] ] , 4 ] ,
"\<,u\>" , NumberForm [ eigenvectors [ [ 1 , 2 ] ] , 4 ] , "\<\]>" ] Print [
"\<Excited state:c\>" , NumberForm [ eigenvectors [ [ 2 , 1 ] ] , 4 ] ,
"\<,u\>" , NumberForm [ eigenvectors [ [ 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\>S\>:2081\>:2081\>" , Simplify [
E1analytical ] ] Print [ "\<,u\>" , N [ E1analytical , 6 ] ] Print [ ]
Print [ "\<E\>:2082\>H\>:2082\>S\>:2082\>:2082\>" , Simplify [
E2analytical ] ] Print [ "\<,u\>" , 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 [ ] \
(* 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 [ evaluates [ [ 1 ] ] - exactE1 ] / exactE1 ; err2 = 100 *
Abs [ evaluates [ [ 2 ] ] - exactE2 ] / exactE2 ; \
Print [ StringForm [ "\<` `` `` `` `` `` `` `` `` \>" , StringPadRight [ "\<E\>:2081\>" ,

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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_ ] := evector [ [ 1 , 1 ] ] * f1 [ x ] + evector [ [ 1 , 2 ] ]
* f2 [ x ] psi2 [ x_ ] := evector [ [ 2 , 1 ] ] * f1 [ x ] + evector
[ [ 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 ] ,

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{ - 2.2 , 4.2 } ] , Text [ Style [ "\<ThickLine:\u2022Potential\u2022V(x)\>" ,
10 ] , { - 2.2 , 3.9 } ] } ] \*
(* === === === = STEP 10 : Comments and Analysis === === === = *) \
Print [ Style [ "\<STEP\u202210:\u2022Analysis\u2022and\u2022Comments\>" , , 14 ] ] Print [ ]
\
Print [ "\<1.\u2022PARITY\u2022SYMMETRY:\u2022\>" ] Print [ "\<\u2022[Bullet]\u2022V(x)\u2022=\u2022g|x|\u2022is\u2022
EVEN:\u2022V(-x)\u2022=\u2022V(x)\u2022\>" ] Print [ "\<\u2022[Bullet]\u2022f\':2081(x)\u2022is\u2022EVEN:\u2022f
\':2081(-x)\u2022=\u2022f\':2081(x)\u2022\>" ] Print [ "\<\u2022[Bullet]\u2022f\':2082(x)\u2022is\u2022ODD:\u2022f
\':2082(-x)\u2022=\u2022-f\':2082(x)\u2022\>" ] Print [ ] Print [ ] \
Print [ "\<2.\u2022BLOCK-DIAGONAL\u2022STRUCTURE:\u2022\>" ] Print [ "\<\u2022[Bullet]\u2022
Hamiltonian\u2022separates\u2022into\u2022even\u2022and\u2022odd\u2022sectors\>" ] Print [ ] Print [
] Print [ ] \
Print [ "\<3.\u2022ACCURACY\u2022OF\u2022RAYLEIGH-RITZ:\u2022\>" ] Print [ "\<\u2022[Bullet]\u2022Ground\u2022
state\u2022error:\u2022\>" , NumberForm [ err1 , { 5 , 2 } ] , "\<%\>" ] Print [
"\<\u2022[Bullet]\u2022Excited\u2022state\u2022error:\u2022\>" , NumberForm [ err2 , { 5 , 2 } ]
, "\<%\>" ] Print [ "\<\u2022[Bullet]\u2022Excellent\u2022for\u2022only\u20222\u2022basis\u2022functions
!\u2022\>" ] Print [ "\<\u2022[Bullet]\u2022RR\u2022method\u2022provides\u2022UPPER\u2022BOUNDS\u2022to\u2022true\u2022
energies\>" ] Print [ ] \
Print [ "\<4.\u2022VARIATIONAL\u2022PRINCIPLE\u2022VERIFICATION:\u2022\>" ] Print [ "\<\u2022[Bullet]
]\u2022E\':2081(RR)\u2022[GreaterEqual]\u2022E\':2081(exact)?\u2022\>" , evaluates [ [ 1 ] ] >=
exactE1 ] Print [ "\<\u2022[Bullet]\u2022E\':2082(RR)\u2022[GreaterEqual]\u2022E\':2082(
exact)?\u2022\>" , evaluates [ [ 2 ] ] >= exactE2 ] Print [ ] Print [ ] \
Print [ "\<5.\u2022PHYSICAL\u2022INTERPRETATION:\u2022\>" ] Print [ "\<\u2022[Bullet]\u2022Linear\u2022
potential\u2022g|x|\u2022is\u2022au'\u2022V-shaped'\u2022well\>" ] Print [ ] Print [ "\<\u2022[Bullet]
]\u2022Ground\u2022state:\u2022concentrated\u2022near\u2022x\u2022=\u20220,\u2022no\u2022nodes\>" ] Print [ "\<\u2022[
Bullet]\u2022Excited\u2022state:\u2022has\u2022node\u2022at\u2022x\u2022=\u20220\u2022(odd\u2022parity)\>" ] Print [ ] \
Print [ "\<6.\u2022WHY\u2022THE\u2022METHOD\u2022WORKS\u2022WELL:\u2022\>" ] Print [ "\<\u2022[Bullet]\u2022
Gaussian\u2022basis\u2022captures\u2022the\u2022localized\u2022nature\>" ] Print [ "\<\u2022[Bullet]\u2022
Parity\u2022structure\u2022exactly\u2022preserved\>" ] Print [ "\<\u2022[Bullet]\u2022
Variational\u2022freedom\u2022via\u2022linear\u2022combinations\>" ] Print [ ] \
In[4731]:= db1085e3-a732-bc42-ba4f-77b237bb4e4d

```

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

STEP 1: Basis Functions

$$f2081(x) = \exp(-x^2/a^2) [\text{EVEN function}] \quad f2082(x) = x \text{CenterDot} \exp(-x^2/a^2) [\text{ODD function}]$$

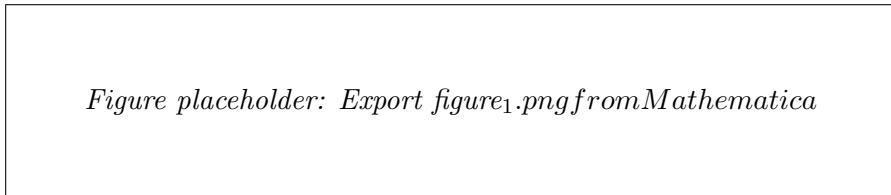


Figure 1: Figure 1

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

$$S20812081 = \int f2081^2 dx = S 2081 2082 = \int f2081 \text{CenterDot} f2082 dx = "", "", "0", "", "" (\text{odd integrand} \rightarrow 0)$$

S 2082 2081 = S 2081 2082 =

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

Overlap Matrix S (symbolic):

Overlap Matrix S (numerical):

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

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

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

$$\mathbf{T 2082 2081 = T 2081 2082 =}$$

$$\mathbf{T 2082 2082 = -\dot{b}d} \int f 2082 \text{CenterDot} f 2082'' dx =$$

Kinetic Energy Matrix T (symbolic):

Kinetic Energy Matrix T (numerical):

$$\text{STEP 4: Potential Energy Matrix } V 1d62 2c7c = g 27e8f 1d62 \text{---x---} f 2c7c 27e9$$

$$V 2081 2081 = g \int |x| \text{CenterDot} f 2081^2 dx = \mathbf{V 2081 2082 = g} \int |x| \text{CenterDot} f 2081 \text{CenterDot} f 2082 dx = (\text{parity} \rightarrow 0)$$

$$\mathbf{V 2082 2081 = V 2081 2082 =}$$

$$V 2082 2082 = g \int |x| \text{CenterDot} f 2082^2 dx =$$

Potential Energy Matrix V (symbolic):

Potential Energy Matrix V (numerical):

$$\text{STEP 5: Hamiltonian Matrix } H = T + V$$

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: $E_{2099} = g^{(2/3)} \text{CenterDot} |\alpha_{2099}|$ where α_{2099} are the zeros of the Airy function $Ai(-z)$.

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[61.55]

E 2082 2.29788 4.08795 RowBox[43.79]

STEP 9: Visualization of Results

Figure placeholder: Export figure2.png from Mathematica

Figure 2: Figure 2

Figure placeholder: Export figure3.png from Mathematica

Figure 3: Figure 3

STEP 10: Analysis and Comments

1. PARITY SYMMETRY:

• $V(x) = g|x|$ is EVEN : $V(-x) = V(x)$ • $27e8 f 2081|O|f 2082 27e9 = 0$ for any even operator O

2. BLOCK-DIAGONAL STRUCTURE:

- Hamiltonian separates into even and odd sectors
- Ground state : EVEN parity (only if $c_{2081}, c_{2081} \neq 0, c_{2082} = 0$)
- First excited : ODD parity (only if $c_{2082}, c_{2081} = 0, c_{2082} \neq 0$)

3. ACCURACY OF RAYLEIGH-RITZ:

- Ground state error : 61.5543.79

4. VARIATIONAL PRINCIPLE VERIFICATION:

- $E_{2081}(RR) \geq E_{2081}(\text{exact})$?
- $E_{2082}(RR) \geq E_{2082}(\text{exact})$?
- Approximate energies are indeed upper bounds ✓

5. PHYSICAL INTERPRETATION:

- Linear potential $g|x|$ is a 'V-shaped' well
- With $g = \hbar^2/(ma) = 1$, length scale set by $a = 1$
- Ground state : concentrated near $x = 0$, no nodes
- Excited state : has node at $x = 0$ (odd parity)

6. WHY THE METHOD WORKS WELL:

- Parity structure exactly preserved