VP390 Bonus Question Set 1

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For the stationery equation $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{x}^2} + V(x)\psi(x) = E\psi(x)$
where

$$V(x) = \begin{cases} V_1 & x \leq a \\ -V_0 & |x| < a \\ V_2 & x \geq a \end{cases}$$

$\frac{\mathrm{d}^2\psi(x)}{\mathrm{x}^2} + \frac{2m}{\hbar^2}(E - V)\psi(x) = 0$, hence we can get equations

$$\psi(x) = \begin{cases} A_1 e^{\kappa_1 x} & \kappa_1^2 = -\frac{2m}{\hbar^2}(E - V_1) & x \leq -a \\ C_1 \cos kx + C_2 \sin kx & k^2 = \frac{2m}{\hbar^2}(E + V_0) & |x| < a \\ A_2 e^{-\kappa_2 x} & \kappa_2^3 = -\frac{2m}{\hbar^2}(E - V_2) & x \geq a \end{cases}$$

Since the derivative and function should be continuous at $x = a$ and $x = -a$, we get:

$$\begin{cases} A_1 e^{-\kappa_1 a} = C_1 \cos ka - C_2 \sin ka & (1) \\ A_2 e^{\kappa_2 a} = C_1 \cos ka + C_2 \sin ka & (2) \\ \kappa_1 A_1 e^{-\kappa_1 a} = kC_1 \sin ka + kC_2 \cos ka & (3) \\ -\kappa_2 A_2 e^{\kappa_2 a} = -kC_1 \sin ka + kC_2 \cos ka & (4) \end{cases}$$

According to a model from mathematica, we can solve the equation graphically[1].

1 Problem 1

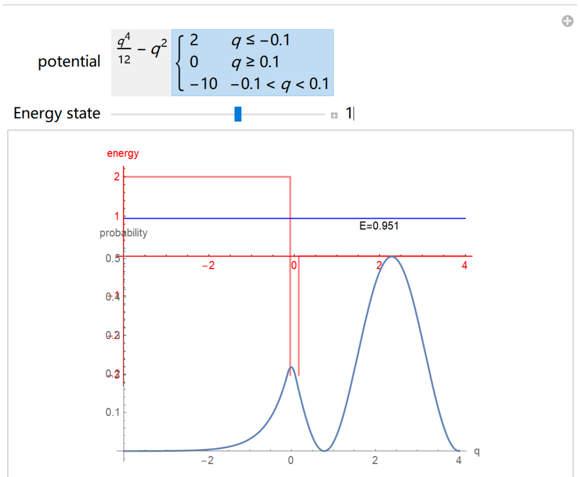


Figure 1: The first state eigenenergy for $a = 0.1$

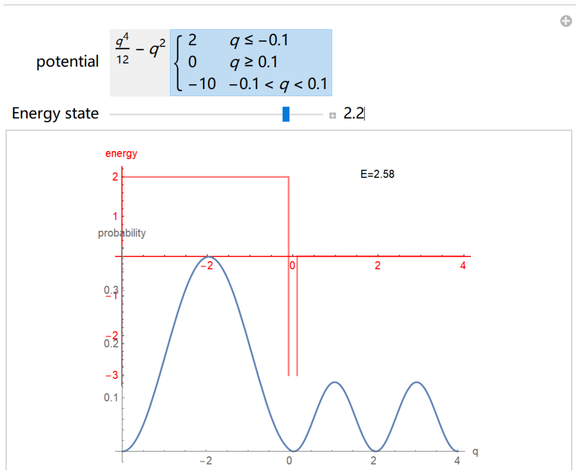


Figure 2: The second state eigenenergy for $a = 0.1$

2 Problem 2

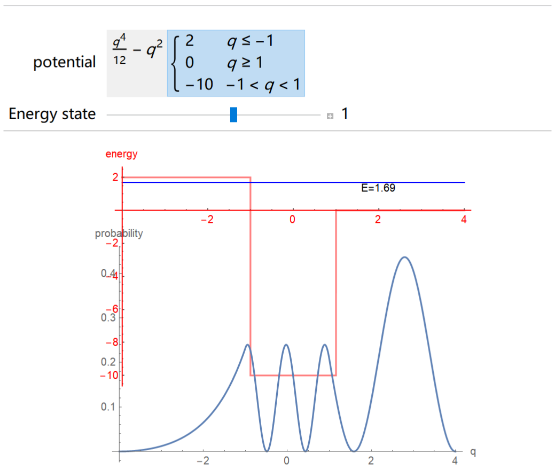


Figure 3: The first state eigenenergy for $a = 1$

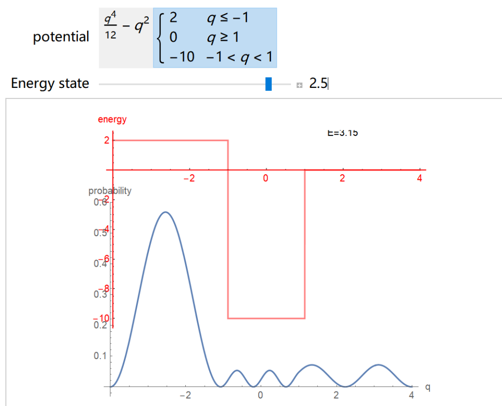


Figure 4: The second state eigenenergy for $a = 2$

References

[1] https://demonstrations.wolfram.com/QuantumWellExplorer/

Modified Mathematica Code

Quantum Well Explorer

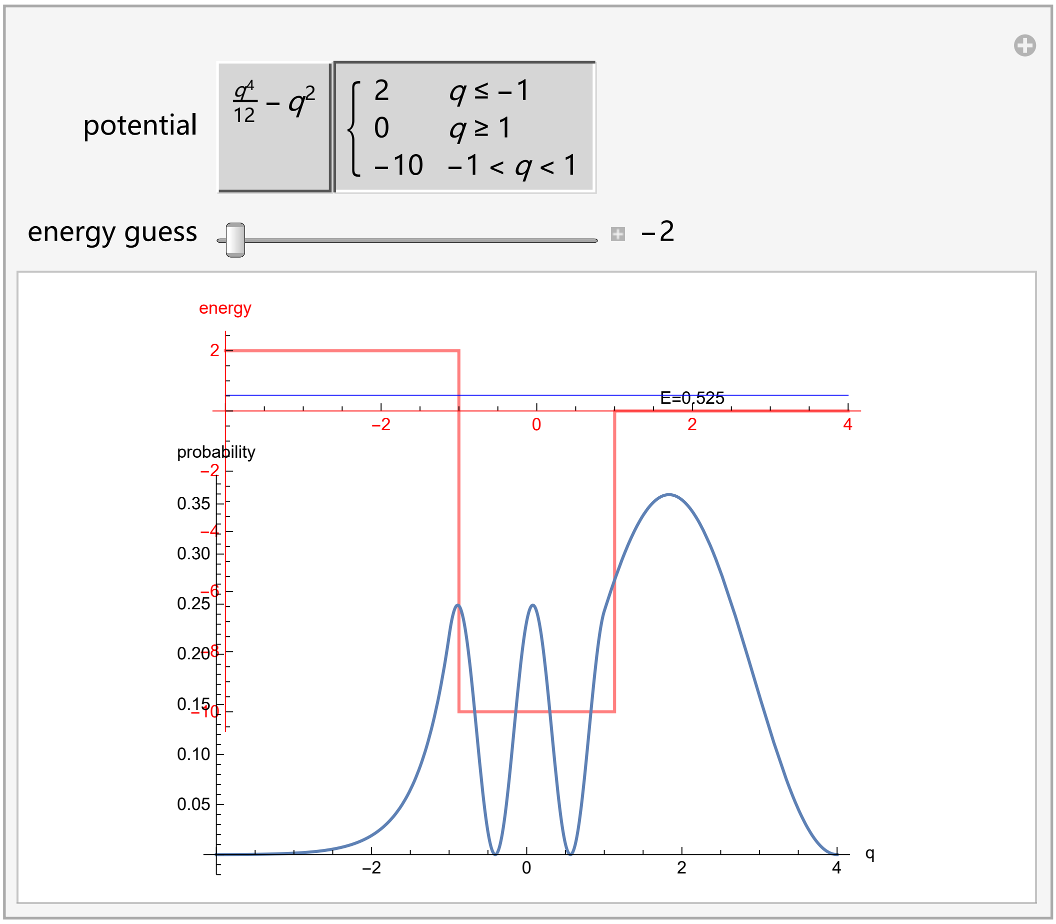
In[4]:=

```
EigenSolver[V_, {q_, qmin_, qmax_}, matchPoint_, EnergyGuess_] :=
 Module[{leftψ, rightψ, scaleLeft, scaledLeft, MatchingPoint, ψ, ϵ, scaleRight,
 模块
   DRight, DLeft, Energy, result, normalization, plot1, plot2, gr},
  Developer`SetSystemOptions["EvaluateNumericalFunctionArgument" → False];
                                                                    假
  MatchingPoint = Rule[q, matchPoint];
                  规则
  leftψ[ϵ_, q] :=
   First[NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == ϵ ψ[q], ψ'[qmin] == 0.0001, ψ[qmin] == 0},
   第一个 数值求解… 偏导
      ψ[q], {q, qmin, q /. MatchingPoint}]][[1, 2]];
  rightψ[ϵ_, q] := First[NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == ϵ ψ[q], ψ'[qmax] ==
                   第一个 数值求解…  偏导
        0.0001, ψ[qmax] == 0}, ψ[q], {q, qmax, q /. MatchingPoint}]][[1, 2]];
  scaleLeft[ϵ_] := leftψ[ϵ, q] /. MatchingPoint;
  scaleRight[ϵ_] := rightψ[ϵ, q] /. MatchingPoint;
  scaledLeft[ϵ_, q] := leftψ[ϵ, q] scaleRight[ϵ] / scaleLeft[ϵ];
  DRight[ϵ_, q] := D[rightψ[ϵ, q], q];
                   偏导
  DLeft[ϵ_, q] := D[scaledLeft[ϵ, q], q];
                  偏导
  Energy =
   ϵ /. FindRoot[(DLeft[ϵ, q] /. MatchingPoint) == (DRight[ϵ, q] /. MatchingPoint),
        求根
     {ϵ, EnergyGuess, EnergyGuess + EnergyGuess / 10.0}];
  result = First[ψ[q] /. NDSolve[{-D[ψ[q], {q, 2}] + V ψ[q] == Energy ψ[q],
           第一个          数值求解…  偏导
      ψ'[qmin] == 0.0001, ψ[qmin] == 0}, ψ[q], {q, qmin, qmax}]];
  normalization = 1 / √NIntegrate[result^2, {q, qmin, qmax}] ;
  plot1 = Show[
          显示
    Plot[Tooltip[V, ToString[TraditionalForm[V]]], {q, qmin, qmax}, PlotPoints → 100,
         提示条      转换为…   传统格式                                      绘图点
     PlotStyle → {RGBColor[1, 0, 0], Opacity[.5]}, AxesOrigin → {qmin, 0},
                  RGB颜色            不透明度       坐标轴原点
     AxesLabel → "energy", Exclusions → None, AxesStyle → Red], Graphics[Text[
                          排除            无     坐标轴样式    红色   图形      文本
      StringJoin["E=", ToString[NumberForm[Energy, 3]]], {qmax / 2, 0.8 Energy}]],
      …          转换为…   数值近似
    Graphics[{RGBColor[0, 0, 1], Line[{{qmin, Energy}, {qmax, Energy}}]}]];
              RGB颜色             线段
  plot2 = Plot[normalization^2 result^2, {q, qmin, qmax}, AxesOrigin → {qmin, 0},
          绘图                                            坐标轴原点
    PlotRange → All, AxesLabel → {"q", "probability"}, RotateLabel → True];
                全部  坐标轴标签                         旋转标签      真
```

```
gr = GraphicsGrid[{{plot1}, {plot2}}, Spacings → Scaled[-1],
     |图形网格                              |间隔        |比例坐标
   ImageSize → {500, 300}];
  |图像尺寸
Developer`SetSystemOptions["EvaluateNumericalFunctionArgument" → True];
                                                                  |真
gr]
```

In[11]:=
```
V0 = -10;
V1 = 2;
V2 = 0;
a = 1;
Manipulate[Quiet[EigenSolver[V, {q, -4, 4}, -3.6, EnergyGuess]],
|交互式操作   |不输出任何消息
 {{V, -q^2 + q^4 / 12, "potential"}, {-q^2 + q^4 / 12 → ToString[-q^2 + q^4 / 12, TraditionalForm],
                                                       |转换为字符串          |传统格式
   Piecewise[{{V1, q <= -a}, {V2, q ≥ a}, {V0, -a < q < a}}] → ToString[
   |分段函数                                                   |转换为字符串
     Piecewise[{{V1, q <= -a}, {V2, q ≥ a}, {V0, -a < q < a}}], TraditionalForm]}},
     |分段函数                                                  |传统格式
 {{EnergyGuess, -2, "energy guess"}, -2, 3, Appearance → "Labeled"},
                                            |外观          |标记
 SaveDefinitions → True, TrackedSymbols :→ {V, EnergyGuess}, ContinuousAction → False]
 |保存定义          |真    |被跟踪的符号                        |连续行为               |假
```

Out[15]=



CAPTION

DETAILS

THIS NOTEBOOK IS THE SOURCE CODE FROM

"Quantum Well Explorer" from the Wolfram Demonstrations Project
http://demonstrations.wolfram.com/QuantumWellExplorer/

- Contributed by: Richard Gass

A full-function Wolfram *Mathematica* system (Version 6 or higher) is required to edit this notebook.

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