Particle in a Potential $U(x) = \mu x^4$

Statement of the problem

Consider the one dimensional motion of a particle of mass m and energy E in a quartic potential

$$U(x) = \mu x^4, \mu > 0. \tag{1}$$

We want to calculate the energy levels and the wave functions of the bound states of such a particle. We will find them in the semiclassical approximation and compare with the exact results obtained by numerically solving the Schrödinger equation.

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right)\psi_n(x) \;=\; E_n\psi_n(x),\; n = 1, 2, ... \tag{2}$$

We consider first the solution of this problem in the semiclassical approximation. Let us define the turning points $x = a_n$ and $x = b_n$, for which $U(x) = E_n^s$, where E_n^s is the energy of the n-th bound state in this approximation, see Fig. .

The equation which will determine the values of E_n^s as a function of n is the Born-Sommerfeld quantization condition

$$\int_{a_n}^{b_n} \sqrt{2m\,(\,E_n^s - U(x)\,)}\,dx \;=\; (n - \frac{1}{2})\,\pi\,\hbar,\; n = 1, 2, ... \tag{3}$$

(a) Calculate E_n^s as a function of n for the potential (1). Express your result using the constant

$$C \;=\; \int_{-1}^{1} \sqrt{1 - z^4}\,dz \tag{4}$$

Use `Mathematica` to evaluate C. Plot E_n^s for $n = 1, 2, \ldots, 7$, for $\hbar\mu^{1/4}/\sqrt{2m} = 1$.

(b) Use the provided `Mathematica` notebook `Quartic.ma` to plot the phase space diagrams ($p(x)$ versus x, where $p(x)$ is the classical momentum of the particle at the coordinate x) for the obtained energy levels. State condition (3) in terms of the areas encompassed by the obtained trajectories in the phase scace.

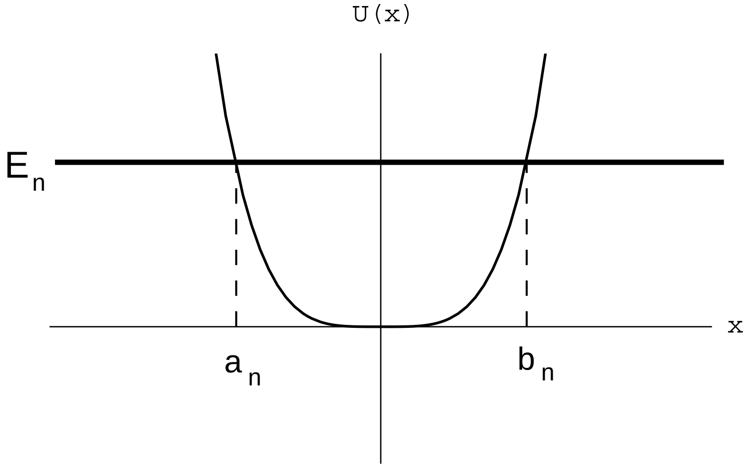


Figure 1: A potential well $U(x) = \mu x^4, \mu > 0$. The points $x = a_n$ and $x = b_n$ are the turning points, i.e., $U(a) = U(b) = E_n^s$. E_n^s is the enrgy of the n-th bound state of the particle in the semiclassical approximation.

We now continue with the numerical sulution of the Schrödinger equation (2) for the potential (1). The numerical methods are discussed in the notebook.

(c) Use the provided `Mathematica` notebook to plot the solutions of the Schrödinger equation (2) for the potential (1) for values of the energy $E = 2, 5, 10, 25$ in units of $\hbar\mu^{1/4}/\sqrt{2m}$. What is the behavior of these solutions at $x \to \infty$? Why?

(d) Numerically compute the first seven bound states of the particle in the potential (1). Plot their energies E_n^e for $n = 1, 2, \ldots, 7$. Plot the relative errors $(E_n^s - E_n^e)/E_n^e$ of the energies determined by the semiclassical and the exact numerical approaches as a function of n. How does this quantity depend on n?

(e) Plot the wave functions $\psi_n(x)$ of the first seven bound states.

Solution

(a) We first find the turning points $x = \pm x_0$, for which $U(x_0) = U(-x_0) = E$, for a given energy E.

$$\mu x_0^4 = E \quad \Longrightarrow \quad x_0 = (E/\mu)^{1/4} . \tag{5}$$

We now apply the Born-Sommerfeld condition

$$\int_{-x_0}^{x_0} \sqrt{2m\,(\,E_n - U(x)\,)}\,dx \;=\; (n - \frac{1}{2})\,\pi\,\hbar,\;\; n = 1, 2, ... \tag{6}$$

to find E_n as a function of n. Substituting $U(x) = \mu x^4$ in (6) one finds

$$\sqrt{2mE_n}\int_{-(E_n/\mu)^{1/4}}^{(E_n/\mu)^{1/4}} \sqrt{1 - \frac{\mu x^4}{E_n}}\,dx \;=\; (n - \frac{1}{2})\,\pi\,\hbar,\;\; n = 1, 2, ... \tag{7}$$

A substitution $z = (\mu/E_n)^{1/4}\,x$ transforms (7) to

$$\sqrt{2mE_n}\left(\frac{E_n}{\mu}\right)^{1/4}\int_{-1}^{1} \sqrt{1 - z^4}\,dz \;=\; (n - \frac{1}{2})\,\pi\,\hbar,\;\; n = 1, 2, ... \tag{8}$$

Using the definition of C

$$C \;=\; \int_{-1}^{1} \sqrt{1 - z^4}\,dz \tag{9}$$

one finally finds

$$E_n \;=\; \left[\frac{\pi}{C}\,\frac{\mu^{1/4}\hbar}{\sqrt{2m}}\,(n - \frac{1}{2})\right]^{4/3},\;\; n = 1, 2, ... \tag{10}$$

The numerical value of C calculated by `Mathematica` is $C = 1.74804$. Fig. 2 shows the first several values of the energy in the semiclassical approximation for a particle in such a quartic potential. The unit for the energy is $\hbar\mu^{1/4}/\sqrt{2m}$.

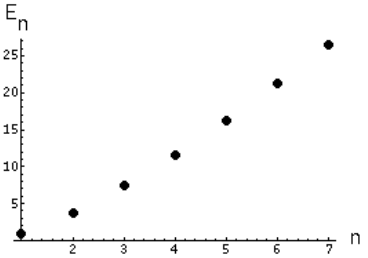


Figure 2: Plot of the semiclassical energies of a particle in a potential well $U(x) = \mu\,x^4$. The unit of the energy is $\mu^{1/3}\hbar^{4/3}(2m)^{-2/3}$.

(b) We plot in Fig.3 the first seven phase space trajectories – $p(x)$ vs. x, where $p(x) = \sqrt{2m(E - U(x))}$ is the classical momentum of the particle at the coordinate x.

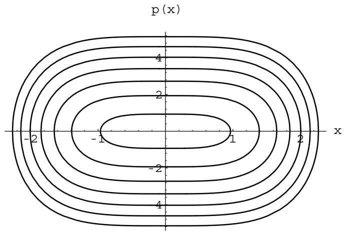


Figure 3: The first seven phase space trajectories of the semiclassical motion. The total energy of the partcicle increases for trajectories further away from the origin.

The integral in the left-hand side of (6) gives the area encompassed by the upper half of any of the closed phase space trajectories and the x axis. Thus (6) is equivalent to the statement that the n-th trajectory encompasses an area of $(2n-1)\pi\hbar$ units. Another corollary of (6) is that the area between any two consecutive trajectories is constant and equal to $2\pi\hbar$.

(c) We use the provided `Mathematica` notebook to calculate solutions of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\mu x^4\right)\psi(x) \;=\; E\,\psi(x), \tag{11}$$

for several values of the energy E. Since (11) is a second order differential equation one needs to supply two boundary conditions in order to solve it. We choose the boundary conditions at a point x, where $U(x) \gg E$, because we expect that there $\psi(x) \to 0$. Such an assumption is justified since the wave function decays exponentially in the classically forbidden region, where $U(x) > E$. Plots of the wave functions calculated under boundary conditions $\psi(x_b) = 0,\ \psi'(x_b) = 1,\ x_b = -3$, for energies $E = 2, 5, 10, 25$ are presented in Fig. 4.

We see that for the chosen energies $\psi(x)$ diverges as $x \to \infty$. This happens because the chosen energy values are not eigen-values of (11). One has to choose specific values of E in order to obtain a solution which is bound for all values of x. These specific values of E are called the eigen-values of the problem. They are the energy levels of the bound states in this potential.

(d) In order to find the exact values of the energies of the bound states we will use as their first approximations the values of E_n obtained by the semiclassical approximation (10). We use a bisection algorithm which starts with these approximate values and sequentially calculates the exact energies with an arbitrary precision. The results of the `Mathematica` calculations are presented in Fig. 5. The continuous curve is the calculated dependance (10) E_n as a function of n in the semiclassical approximation.

The relative errors of the energy $(E_n^s - E_n^e)/E_n^e$, where the upper indices "s" and "e" denote respectively the *semiclassical* and *exact* energy values, are plotted in Fig. 6. One can see that as n increases the semiclassical approximation is getting better and for sufficiently large n this approximation is quite accurate.

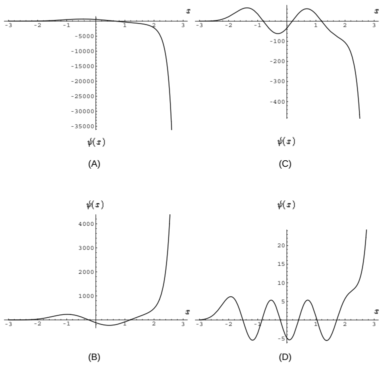


Figure 4: Plots of several general solutions of (11). The boundary conditions were chosen as $\psi(x_b) = 0$, $\psi'(x_b) = 1$, $x_b = -3$. The solutions were calculated for energies: (A) – $E = 2$; (B) – $E = 5$; (C) – $E = 10$; (D) – $E = 25$. The unit of the energy is $\mu^{1/3}\hbar^{4/3}(2m)^{-2/3}$.

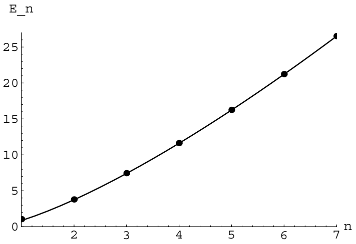


Figure 5: Plot of the energy values of the first seven bound states of a particle in a potential $U(x) = \mu x^4$. The continuous curve is the semiclassically calculated dependance of E_n as a function of n. The dots denote the calculated exact energy values E_n. The unit of the energy is $\mu^{1/3}\hbar^{4/3}(2m)^{-2/3}$.

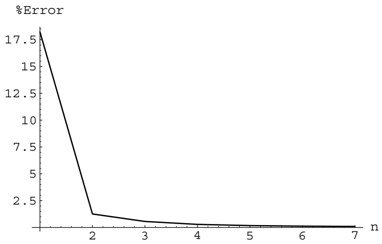


Figure 6: Plot of the relative error in estimation of the energy values of the first seven bound states of a particle in a potential $U(x) = \mu x^4$. The quantity plotted is $(E_n^s - E_n^e)/E_n^e$, where the upper indices denote the semiclassical and exact energy values.

(e) The wave functions of the first four bound states are presented in Fig. 7. One verifies that, indeed, when E is an eigen-value of (11) the corresponding solution is finite. Note the parity of the wave functions.

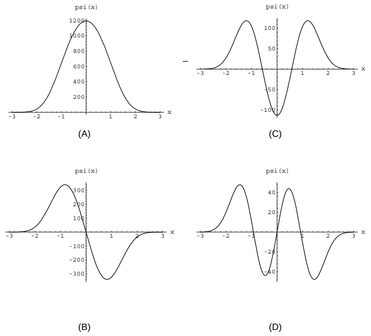


Figure 7: These generated by `Mathematica` plots represent the wave functions of the first four bound states of a paprticle in a potential $U(x) = \mu x^4$. The wave functions are not normalized. The corresponding energy values are: (A) – $E = 1.06036$; (B) – $E = 3.79967$; (C) – $E = 7.4557$; (D) – $E = 11.6448$. The unit of the energy is $\mu^{1/3}\hbar^{4/3}(2m)^{-2/3}$.

□ Particle in a Quartic Potential Well

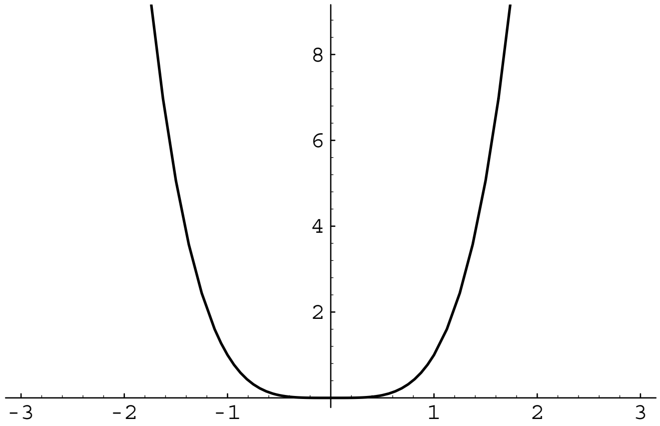
Definiton of the Parameters and the Potential

Here we define some constants and parameters of the problem.

```
In[1]:=     m=1/2;
            hbar=1;
            mu=1;
            nmin=1;
            nmax=7;
            xmin=-3;
            xmax=-xmin;
```

The form of the potentail and the classical momentum p(x) are defined here.

```
In[2]:=     V[x_]=mu x^ 4;
            k2[x_,e_]:=2m/hbar^ 2 (e-V[x]);
            p[x_,e_]:=Sqrt[ Abs[k2[x,e]] ];
            Plot[V[x],{x,xmin,xmax}];
```

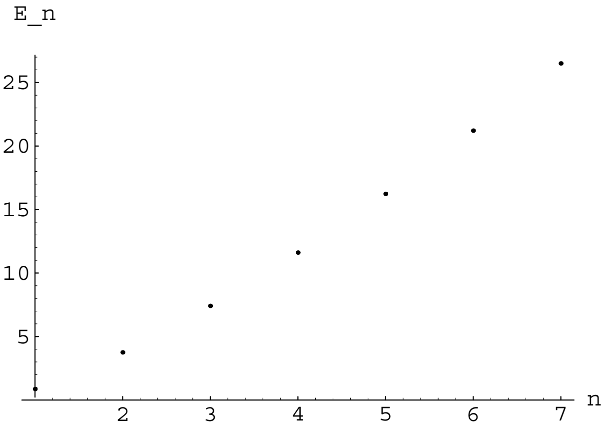


Energy Levels - Semiclassical Approximation

Calculation of the constant C and the semiclassical energies.

```
In[3]:=    c=NIntegrate[Sqrt[1-z^4], {z,-1,1}];
           Print["C= ",c]
           ee[n_]:=(Pi/c(n-1/2))^(4/3)
           semi={};
           Do[ semi = Append[semi, N[ ee[i] ] ], {i, nmin, nmax}]
           semi
           plsemi=ListPlot[semi, AxesLabel->{"n","E_n"}];
```

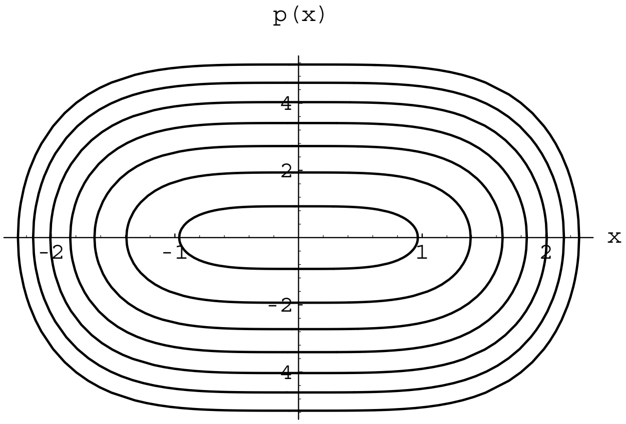
```
C= 1.74804
Out[3]=    {0.867145, 3.75192, 7.41399, 11.6115, 16.2336,
              21.2137, 26.5063}
```



Phase Space Trajectories

Here we create plots of the phase space trajectories for the calculated energy values . Later we show these plots together.

```
In[4]:=   pl=Table[0,{i,nmin,nmax}];
          Do[ e=semi[[i]];
                 x0=(e/mu)^(1/4);
                 pl[[i]]=Plot[ {p[x,e], -p[x,e]}, {x, -x0, x0},
                         DisplayFunction->Identity],
                 {i, nmin, nmax}]

          Show[ pl[[1]], pl[[2]] ,pl[[3]], pl[[4]], pl[[5]], pl[[6]],
          pl[[7]],
          DisplayFunction->$DisplayFunction,
          AxesLabel->{"x","p(x)"}];
```



Numerical Solution of the Schroedinger Equation - the Algorithm

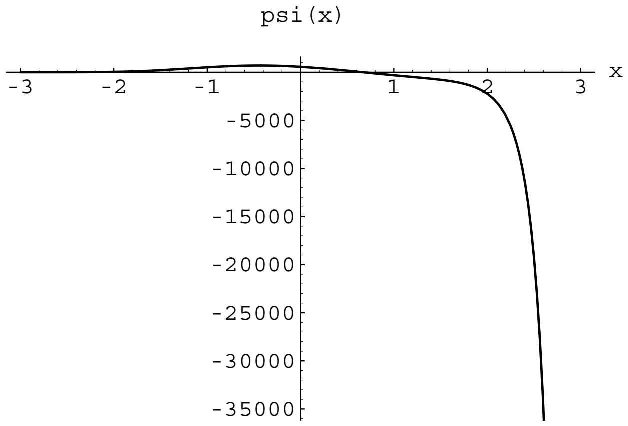
We define four types of routines. They solve the Schroedinger equation for the already inputed form of the potential. The four routines differ in terms of their boundary conditions and if they plot or not the found solutions. All routines return as their output the value of the calculated wave function at x=x_max. This value is used in the bissection algorithm from the next section. The routines called "even" calculate the wave functions with boundary conditions which assure that a stationary soluiton would have an even parity; the "odd" named routines calculate odd solutions. In fact, the only difference in the boundary conditions is the value of the first derivative of the wave function at x=x_min. For the "even" routines it is +1 and for the "odd" ones it is -1. Note that the found solutions are not normalized, so the actual magnitude of the first derivative is not important, only its sign matters. We need this distinction between "even" and "odd" routines for the bissection algorithm routine below.

```
In[5]:=  even[e_]:=Module[ {r,a,y,z},
                 r = NDSolve[{y''[x] == - k2[x,e] y[x], y'[xmin] == 1,
                 y[xmin] == 0}, y, {x, xmin, xmax}];

                 z[x_]=y[x] /. r;
         (*      Plot[z[x], {x, xmin, xmax}];*)
                 a=(y[xmax] /. r)[[1]];
                 Return[a]
                                         ]


                 odd[e_]:=Module[ {r,a,y,z},
                 r = NDSolve[{y''[x] == - k2[x,e] y[x], y'[xmin] == -1,
                 y[xmin] == 0}, y, {x, xmin, xmax}];

                 z[x_]=y[x] /. r;
         (*      Plot[z[x], {x, xmin, xmax}];*)
                 a=(y[xmax] /. r)[[1]];
                 Return[a]
                                         ]


                 evenplot[e_]:=Module[ {r,a,y,z},
                 r = NDSolve[{y''[x] == - k2[x,e] y[x], y'[xmin] == 1,
                 y[xmin] == 0}, y, {x, xmin, xmax}];

                 z[x_]=y[x] /. r;
                 Plot[z[x], {x, xmin, xmax},
                         AxesLabel->{"x","psi(x)"}];
                 a=(y[xmax] /. r)[[1]];
                 Return[a]
                                         ]


                 oddplot[e_]:=Module[ {r,a,y,z},
                 r = NDSolve[{y''[x] == - k2[x,e] y[x], y'[xmin] == -1,
                 y[xmin] == 0}, y, {x, xmin, xmax}];

                 z[x_]=y[x] /. r;
                 Plot[z[x], {x, xmin, xmax}];
                 a=(y[xmax] /. r)[[1]];
                 Return[a]
                                         ]
```

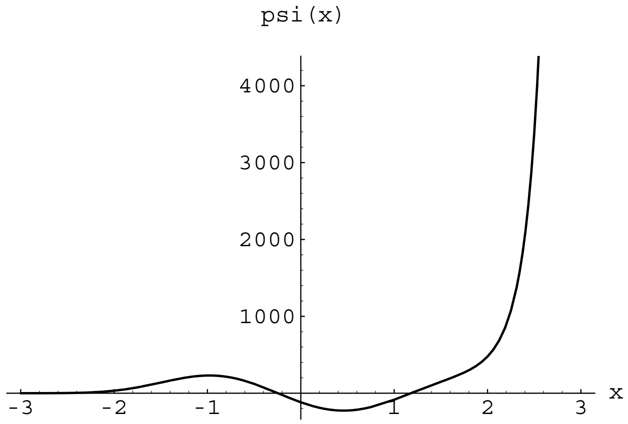
Some Solutions of the Schroedinger Equation

We plot here solution of the Schroedinger equation for several values of the energy with boundary conditions which would have produced even solutions. One can experiment with the "odd" routine to see that the only difference is an unimportant factor of -1.

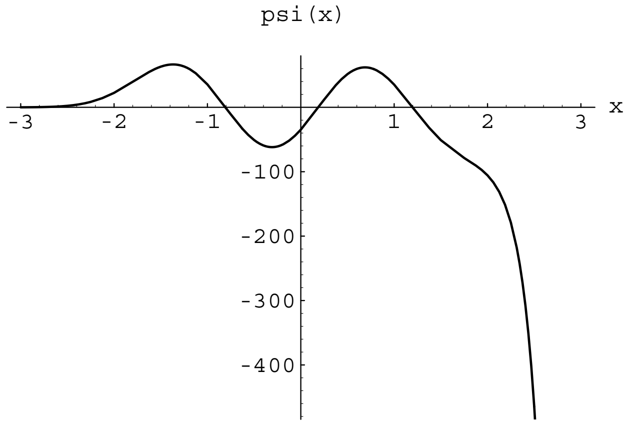
```
In[6]:=  evenplot[2]
         evenplot[5]
         evenplot[10]
         evenplot[25]
          oddplot[25]
```



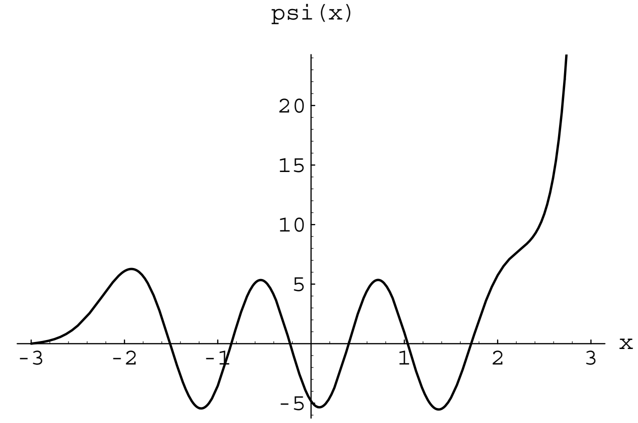
```
Out[6]=     -652198.
```



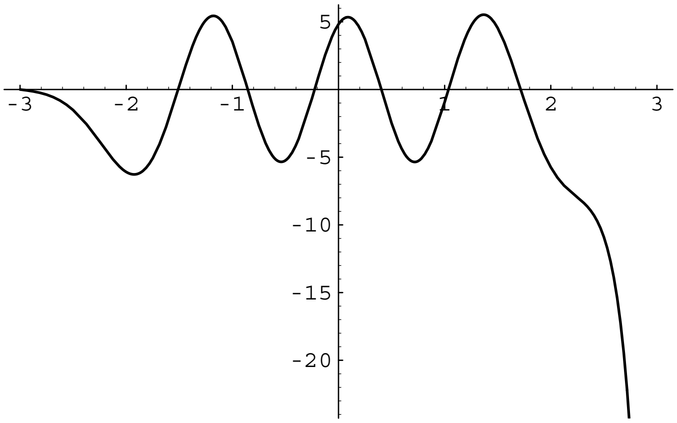
```
Out[6]=     101515.
```



```
Out[6]=     -11236.2
```



```
Out[6]=     110.938
```



```
Out[6]=     -110.938
```

Energy Levels of the Bound States

A bissection algorithm for evaluation of the eigen-values of the Schroedinger equation is realized here.

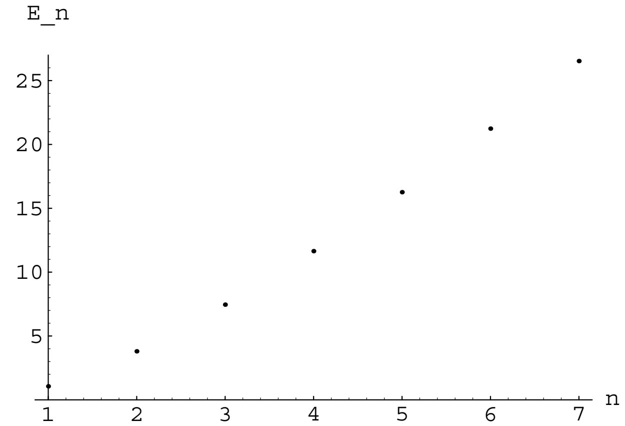
The idea of the algorithm is the following. One starts with some guess value for the true eigen value and solves the Schroedinger equation. Depending on the sign of the calculated wave function at x=x_max. one increases or decreases the guess value of the energy. This is done in such a way as to ensure that the wave function at x=x_max equals zero. Running through several iterations and sequentially decreasing the adjustment step of the energy leads to increasingly more accurate estimates of the eigen-values, of course, within the numerical accuracy of this calculation.

```
In[7]:=   exact={};
          Do[ Print["level= ",i];
                  tail[e_]:=If[EvenQ[i], odd[e], even[e]];
                  guess=semi[[i]];
                  e=guess; Print["guess value= ",e];
                  interval=2;

                  For[    it=1, it<32, it++,
                          a=tail[e];
          (*              Print["exact=",N[e], "   accuracy= ",a];*)
                          interval=interval/2;
                          If[a>0, e=e+interval, e=e-interval]
                          ];
                  exact=Append[exact,e];
                  Print["exact value= ", e];

                  ,{i, nmin, nmax}]
```

```
level= 1
guess value= 0.867145
exact value= 1.06036
level= 2
guess value= 3.75192
exact value= 3.79967
level= 3
guess value= 7.41399
exact value= 7.4557
level= 4
guess value= 11.6115
exact value= 11.6448
level= 5
guess value= 16.2336
exact value= 16.262
level= 6
guess value= 21.2137
exact value= 21.239
level= 7
guess value= 26.5063
exact value= 26.5308
```

Here we plot the values of the calculated eigen-values.

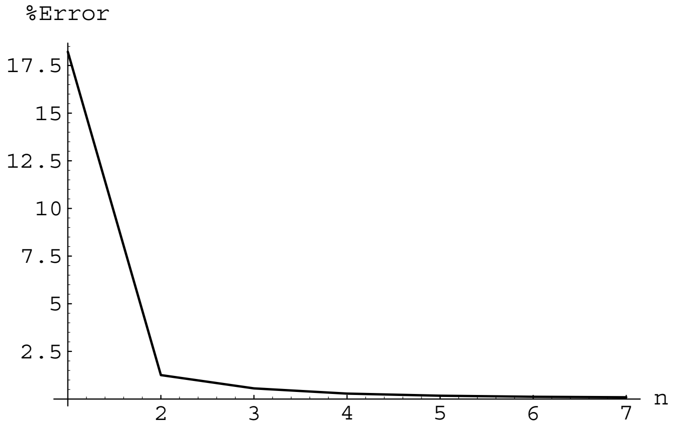
```
In[8]:=   exact
          plexact=ListPlot[exact, AxesLabel->{"n","E_n"},
                  PlotRange->{0,27}]

Out[8]=   {1.06036, 3.79967, 7.4557, 11.6448, 16.262, 21.239,

            26.5308}
```



```
Out[8]=    -Graphics-
```

Here we plot the relative errors of the semiclassically calculated energy levels and the corresponding numerically obtained eigen-values.

```
In[9]:=    exact-semi
           procenterror=100 (exact-semi)/exact
           ListPlot[procenterror, PlotJoined -> True,
           AxesLabel->{"n","%Error"}]
Out[9]=    {0.193217, 0.0477528, 0.0417105, 0.0332484, 0.028344,
             0.025318, 0.0244734}
Out[9]=    {18.2218, 1.25676, 0.559444, 0.285522, 0.174296,
             0.119205, 0.0922452}
```

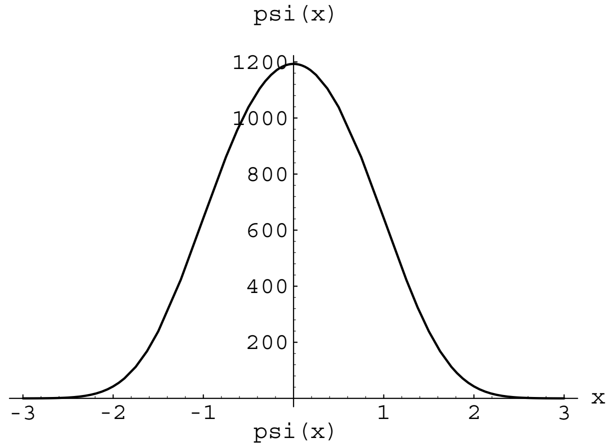


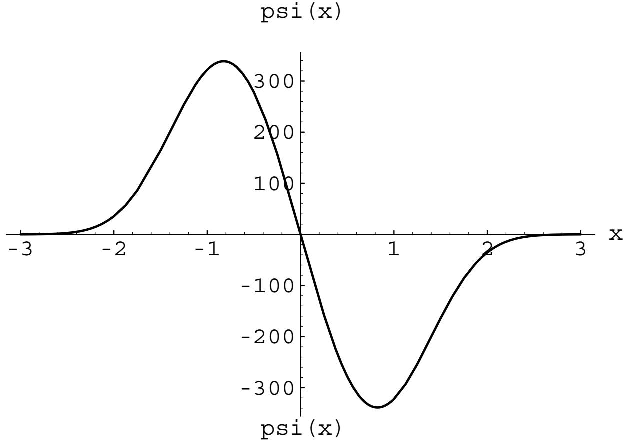
```
Out[9]=    -Graphics-
```

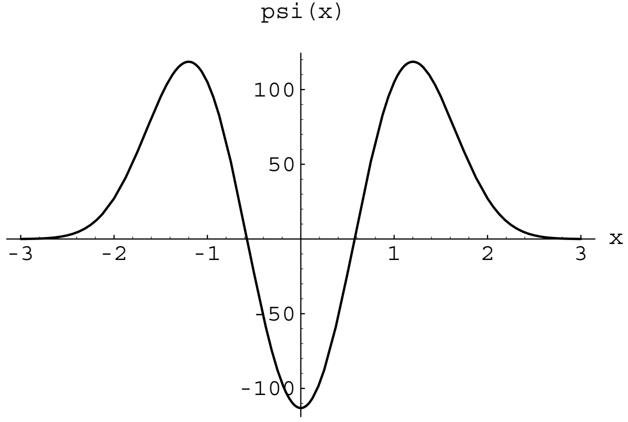
Wave Functions of the Bound States

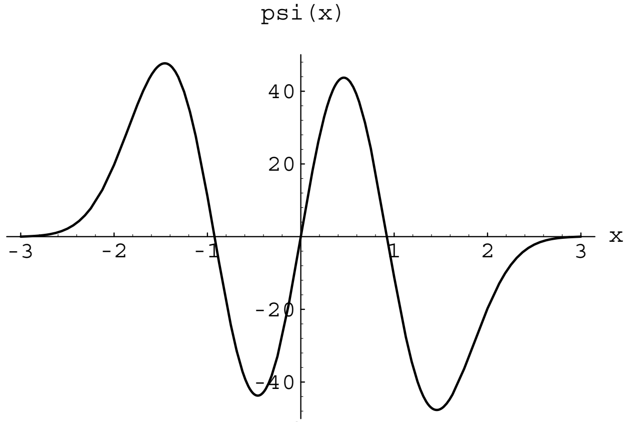
The first seven eigen states are plotted. Note that they are not normalized.

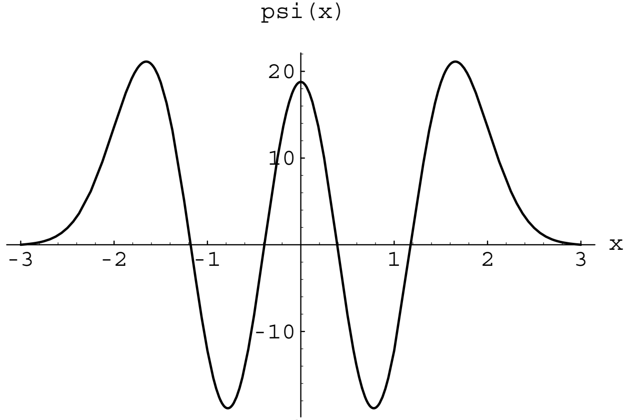
```
In[10]:=    Do[evenplot[exact[[i]]], {i,nmin, nmax}]
```

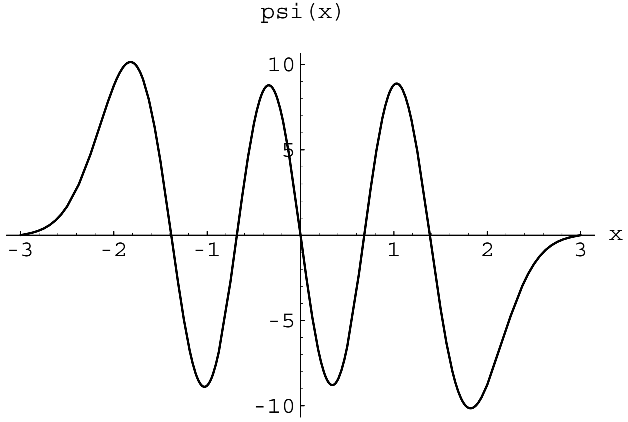


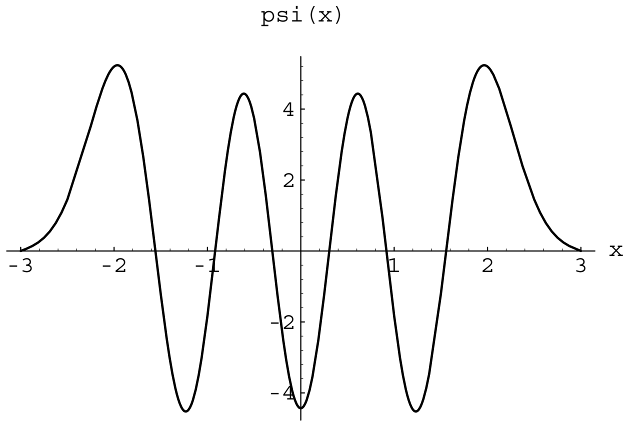





psi(x)
40
20
-20
-40
-3
-2
-1
1
2
3
x


psi(x)
20
10
-10
-3
-2
-1
1
2
3
x


psi(x)
10
5
-5
-10
-3
-2
-1
1
2
3
x


psi(x)
x
4
2
-2
-4
-3
-2
-1
1
2
3