

```

In[ ]:= SetDirectory[NotebookDirectory[]];
Import["init.wl"];

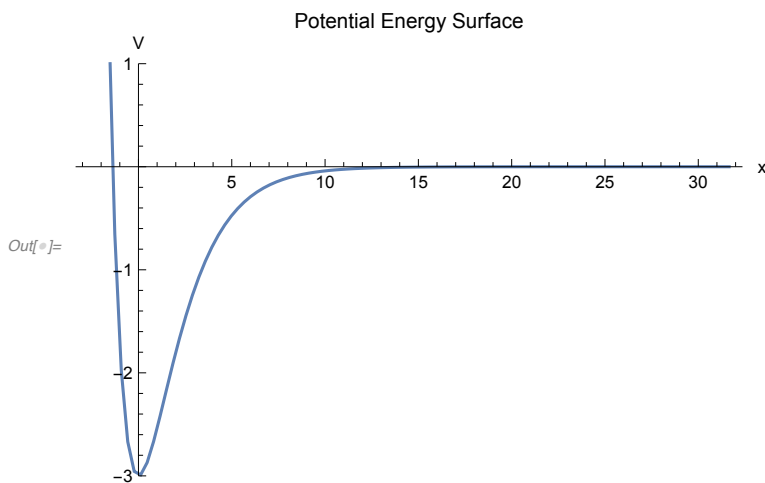
In[ ]:= tcheby[npts_, xmin_, xmax_] := Module[{pts, fb, del}, del = xmax - xmin;
  pts = N[Table[ $\frac{i \text{ del}}{npts + 1} + \text{xmin}$ , {i, npts}]];
  fbrke = N[Table[ $\left(\frac{i \pi}{\text{del}}\right)^2$ , {i, npts}]];
  w = N[Table[ $\frac{\text{del}}{npts + 1}$ , {i, npts}]];
  T = N[Table[ $\sqrt{\frac{2.}{npts + 1}} \sin\left[\frac{(i j) \pi}{npts + 1}\right]$ , {i, npts}, {j, npts}]];
  Return[{pts, T, fbrke, w}]]

dv2fb[DVR_, T_] := T.DVR.Transpose[T];
fb2dv[FBR_, T_] := Transpose[T].FBR.T;

In[ ]:= npts = 100;
xmin = -3.0;
xmax = +32.0;
De = 3.0;
a = .5;
m = 1.0;
ħ = 1.0;
{pts, T, fbrke, w} = tcheby[npts, xmin, xmax];
V[x_] := De (1 - Exp[- a x])^2 - De;
Vdvr = V[pts] // Thread;
fbrke = fbrke *  $\frac{\hbar^2}{2 m}$ ;
Hdvr = fb2dv[DiagonalMatrix[fbrke], T] + DiagonalMatrix[Vdvr];

In[ ]:= plotV = ListPlot[Transpose[{pts, Vdvr}], PlotRange → {-3, 1}, Joined → True,
  AxesLabel → {"x", "V"}, PlotLabel → "Potential Energy Surface"]

```



```

In[ ]:= {ω, φ} = Transpose[Sort[Transpose[Eigensystem[Hdvr]]]];

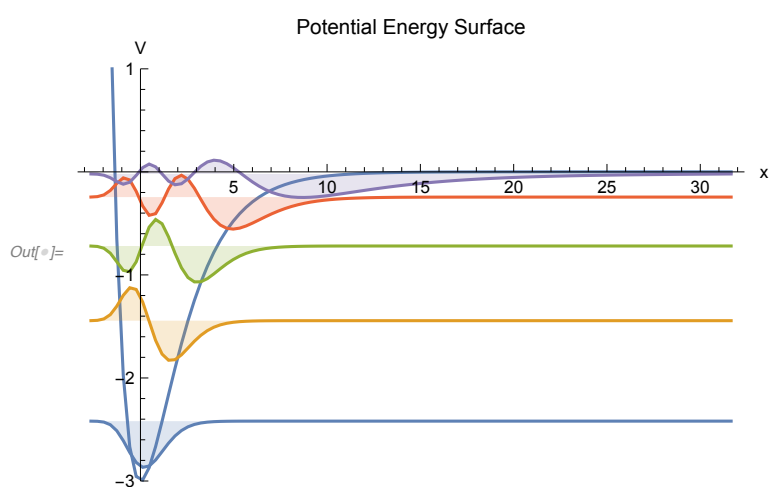
```

```
In[ ]:= TableForm[Take[ $\omega$ , 10]]
```

```
Out[ ]//TableForm=
```

```
-2.41888
-1.44413
-0.719388
-0.244643
-0.0198923
0.0113421
0.0400867
0.0823905
0.136925
0.202919
```

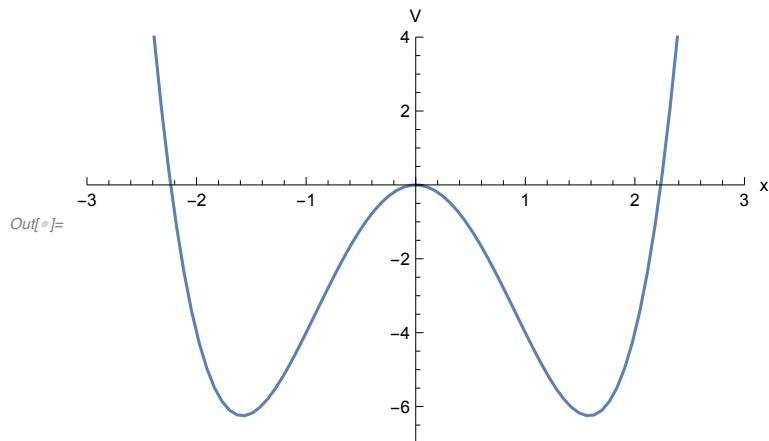
```
In[ ]:= pltWF = ListPlot[Table[Transpose[{pts,  $\omega$ [[i]] +  $\phi$ [[i]]}], {i, 1, 5}],
  PlotRange -> {{-3, 32}, {-3, 1}}, Joined -> True,
  Filling -> Table[i ->  $\omega$ [[i]], {i, 1, 5}]];
Show[plotV, pltWF]
```



```

In[ ]:= {pts2, T2, fbrke2, w2} = tcheby[100, -3.5`, 3.5`];
V2[x_] := -5 x^2 + x^4;
Vdvr2 = Thread[V2[pts2]];
m = 1.`;
pltV = ListPlot[Transpose[{pts2, Vdvr2}],
  PlotRange -> {{-3, 3}, {-7, 4}}, Joined -> True, AxesLabel -> {"x", "V"}]
fbrke2 =  $\frac{\text{fbrke2}}{2 m}$ ;
Hdvr = fb2dv[DiagonalMatrix[fbrke2], T2] + DiagonalMatrix[Vdvr2];
{ $\omega$ ,  $\psi$ } = Transpose[Sort[Transpose[Eigensystem[Hdvr]]]];

```



```

In[ ]:= TableForm[Take[ $\omega$ , 10]]

```

Out[]//TableForm=

```

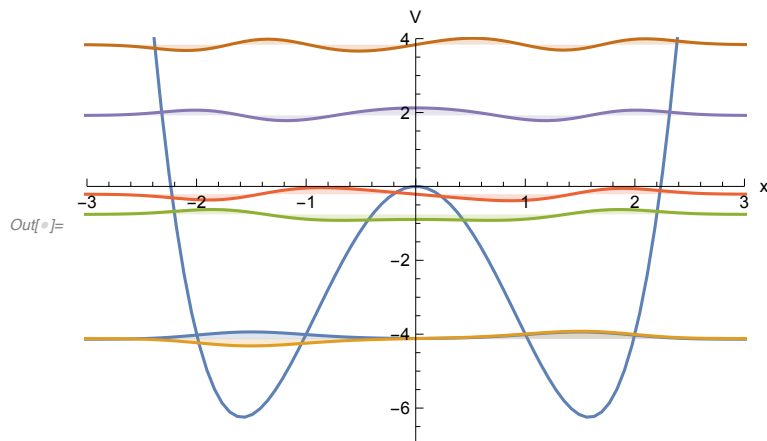
-4.13576
-4.11911
-0.756761
-0.210676
1.92129
3.8373
6.18057
8.7403
11.5102
14.4645

```

```

In[ ]:= nn = 10;
pltWF =
  ListPlot[Table[Transpose[{pts2,  $\omega[[i]] + \psi[[i]]$ }], {i, 1, nn}], Joined → True,
  Filling → Table[i →  $\omega[[i]]$ , {i, 1, nn}]];
Show[pltV, pltWF]

```



```

In[ ]:= npts = 25;
xmin = -3.5;
xmax = 3.5;
params = {A → 1, B → -5, xo → 1.5,  $\beta$  → 0.5,  $\hbar$  → 1,  $\delta t$  → 0.1, m → 1};

V[x_] := -5 x2 + x4;

tcheby[npts_, xmin_, xmax_] := Module[{pts, fb, del}, del = xmax - xmin;
  pts = Table[i * del * (1 / (npts + 1)) + xmin, {i, npts}] // N;
  fbrke = Table[(i * (Pi / del)) ^ 2, {i, npts}] // N;
  w = Table[del / (npts + 1), {i, npts}] // N;
  T = Table[
    Sqrt[2.0 / (npts + 1)] * Sin[(i * j) * Pi / (npts + 1)], {i, npts}, {j, npts}] // N;
  Return[{pts, T, fbrke, w}];

{pts, T, fbrke, w} = tcheby[npts, xmin, xmax];

fbrke = fbrke / (2 m);

ExpV = (Exp[- $\frac{i}{\hbar}$  V[pts]  $\delta t$  /  $\hbar$ ] /. params) // Thread;
ExpK = (Exp[- $\frac{i}{\hbar}$  fbrke  $\delta t$  / 2] /. params) // Thread;
TT = Transpose[T];

UK = T.DiagonalMatrix[ExpK].TT;
U = UK.DiagonalMatrix[ExpV].UK;

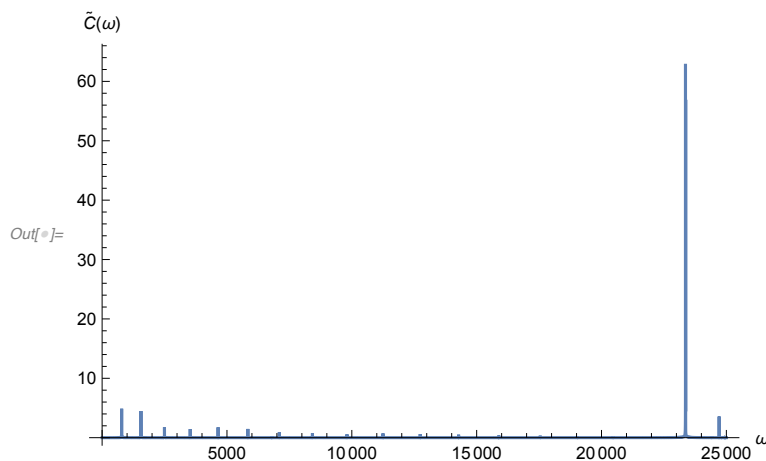
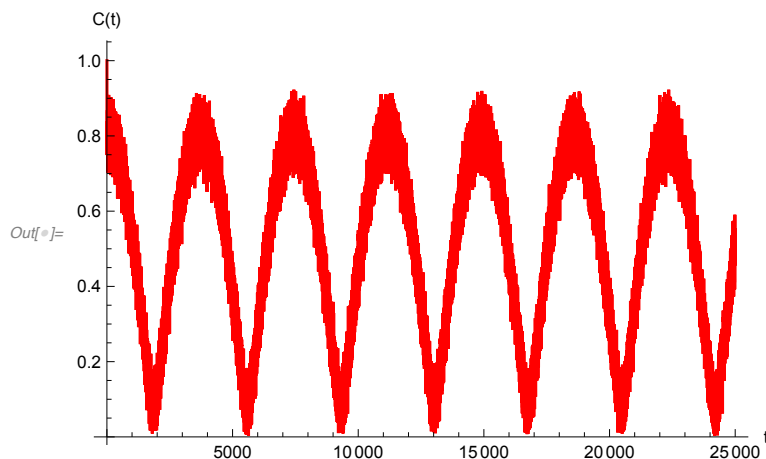
```

```

In[ ]:=  $\psi_0[x_] := \left(\frac{\beta}{\pi}\right)^{1/4} e^{-\beta (x-x_0)^2}; \phi_0 = \text{Thread}[\psi_0[\text{pts}] /. \text{params}];$ 
norm =  $\sqrt{\phi_0 \cdot \phi_0}$ ;
 $\phi_0 = \frac{\phi_0}{\text{norm}}; \psi_t = \{\phi_0\}; \text{ct} = \{1\};$ 
evolve =
{ListPlot[Transpose[{pts,  $\phi_0$ }], Joined → True, DisplayFunction → Identity]};
nsteps = 25 000;
 $\phi_t = \phi_0;$ 
Do[ $\phi_t = U \cdot \phi_t;$ 
c =  $\phi_0 \cdot \phi_t;$ 
ct = Append[ct, c];
If[Mod[n, 1000] == 0,  $\psi_t = \text{Append}[\psi_t, \phi_t];$ 
pp = ListPlot[Transpose[{pts, Abs[ $\phi_t$ ]}],
Joined → True, DisplayFunction → Identity];
evolve = Append[evolve, pp]], {n, nsteps}]; ct1 = ct;

In[ ]:= correl1 = ListPlot[Abs[ct1], Joined → True,
PlotStyle → RGBColor[1, 0, 0], AxesLabel → {"t", "C(t)"}]
cft1 = Fourier[ct];
ct1plot = ListPlot[Abs[cft1], PlotRange → All, Joined → True,
AxesLabel → {" $\omega$ ", " $\sqrt{\frac{1}{2\pi}} \overline{C(\omega)}$ "}]

```



```

In[ ]:= ListPlot[Transpose[{pts, - $\frac{\psi[[1]] + \psi[[2]]}{\sqrt{2}}$ }], Joined → True]

 $\phi_0 = -\frac{\psi[[1]] + \psi[[2]]}{\sqrt{2}};$ 
 $\psi_t = \{\phi_0\};$ 
ct = {1};
evolve =
  {ListPlot[Transpose[{pts,  $\phi_0$ }], Joined → True, DisplayFunction → Identity]};
nsteps = 25 000;
 $\phi_t = \phi_0;$ 
Do[ $\phi_t = U.\phi_t;$ 
  c =  $\phi_0.\phi_t;$ 
  ct = Append[ct, c];
  If[Mod[n, 10 000] == 0,  $\psi_t = \text{Append}[\psi_t, \phi_t];$ 
  pp = ListPlot[Transpose[{pts, Abs[ $\phi_t$ ]}],
    Joined → True, DisplayFunction → Identity];
  evolve = Append[evolve, pp]], {n, nsteps}];
ct2 = ct;

Transpose::nmtx : The first two levels of
{{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538, <<12>>, 1.88462, 2.15385, 2.42308,
2.69231, 2.96154, 3.23077}, {<<23>>, <<49>>, <<50>>}} cannot be transposed.

ListPlot::lpm :
Transpose[{{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538, <<12>>, 1.88462, 2.15385,
2.42308, 2.69231, 2.96154, 3.23077}, {<<1>>}}] is not a list of numbers or pairs of numbers.

Out[ ]:= ListPlot[Transpose[
  {{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538,
    -1.34615, -1.07692, -0.807692, -0.538462, -0.269231, 0., 0.269231,
    0.538462, 0.807692, 1.07692, 1.34615, 1.61538,
    1.88462, 2.15385, 2.42308, 2.69231, 2.96154, 3.23077},
  {2.68424 × 10-8, 7.59465 × 10-8, 1.81563 × 10-7, 4.07246 × 10-7, 8.71183 × 10-7,
    1.7839 × 10-6, 3.50164 × 10-6, 6.59556 × 10-6, 0.000011932, 0.0000207511,
    0.0000347232, 0.0000559529, 0.0000868997, 0.000130187, 0.000188289,
    0.000263102, 0.000355461, 0.000464652, 0.000588045, 0.000720907,
    0.000856506, 0.000986493, 0.00110157, 0.00119234, 0.00125022, 0.00126828,
    0.00124189, 0.00116904, 0.00105038, 0.000888862, 0.000689205, 0.000457126,
    0.00019854, -0.0000812326, -0.000378163, -0.000690088, -0.00101714,
    -0.0013621, -0.0017306, -0.00213143, -0.00257676, -0.00308252, -0.00366893,
    -0.00436112, -0.00519008, -0.00619369, -0.0074181, -0.00891916, -0.010764,
    -0.0130329, -0.0158204, -0.0192366, -0.0234078, -0.0284755, -0.034594,
    -0.0419264, -0.0506368, -0.0608799, -0.0727863, -0.0864447, -0.10188,
    -0.119028, -0.137714, -0.157629, -0.178313, -0.199153, -0.219387,
    -0.238138, -0.254454, -0.267379, -0.27603, -0.279688, -0.277879, -0.270447,
    -0.25759, -0.239873, -0.21818, -0.193649, -0.167557, -0.141202, -0.11578,
    -0.0922828, -0.0714319, -0.053645, -0.0390498, -0.0275261, -0.0187713,
    -0.0123723, -0.00787416, -0.00483435, -0.00286049, -0.00162967,
    -0.000893095, -0.000470352, -0.000237822, -0.000115325, -0.0000535545,
    -0.0000237302, -9.87218 × 10-6, -3.47479 × 10-6}}], Joined → True]

```

Transpose::nmtx : The first two levels of

$\{\{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538, \ll 12 \gg, 1.88462, 2.15385, 2.42308, 2.69231, 2.96154, 3.23077\}, \{\ll 23 \gg, \ll 49 \gg, \ll 50 \gg\}\}$ cannot be transposed.

ListPlot::lpln :

Transpose[$\{\{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538, \ll 12 \gg, 1.88462, 2.15385, 2.42308, 2.69231, 2.96154, 3.23077\}, \{\ll 1 \gg\}\}$] is not a list of numbers or pairs of numbers.

Dot::dotsh : Tensors $\{\{-0.031814 - 0.850043 i, 0.234321 + 0.399686 i, -0.196319 - 0.087358 i, \ll 20 \gg, 0.000277561 - 0.000157053 i, -0.0000789106 + 0.000183584 i\}, \ll 23 \gg, \{\ll 1 \gg\}\}$ and $\{2.68424 \times 10^{-8}, 7.59465 \times 10^{-8}, 1.81563 \times 10^{-7}, 4.07246 \times 10^{-7}, 8.71183 \times 10^{-7}, 1.7839 \times 10^{-6}, \ll 39 \gg, -0.00619369, -0.0074181, -0.00891916, -0.010764, -0.0130329, \ll 50 \gg\}$ have incompatible shapes.

Dot::dotsh : Tensors

$\{2.68424 \times 10^{-8}, 7.59465 \times 10^{-8}, 1.81563 \times 10^{-7}, 4.07246 \times 10^{-7}, 8.71183 \times 10^{-7}, 1.7839 \times 10^{-6}, \ll 39 \gg, -0.00619369, -0.0074181, -0.00891916, -0.010764, -0.0130329, \ll 50 \gg\}$ and $\{\{-0.031814 - 0.850043 i, 0.234321 + 0.399686 i, -0.196319 - 0.087358 i, \ll 20 \gg, 0.000277561 - 0.000157053 i, -0.0000789106 + 0.000183584 i\}, \ll 23 \gg, \{\ll 1 \gg\}\}$ have incompatible shapes.

Dot::dotsh : Tensors $\{\{-0.031814 - 0.850043 i, 0.234321 + 0.399686 i, -0.196319 - 0.087358 i, \ll 20 \gg, 0.000277561 - 0.000157053 i, -0.0000789106 + 0.000183584 i\}, \ll 23 \gg, \{\ll 1 \gg\}\}$ and $\{2.68424 \times 10^{-8}, 7.59465 \times 10^{-8}, 1.81563 \times 10^{-7}, 4.07246 \times 10^{-7}, 8.71183 \times 10^{-7}, 1.7839 \times 10^{-6}, \ll 39 \gg, -0.00619369, -0.0074181, -0.00891916, -0.010764, -0.0130329, \ll 50 \gg\}$ have incompatible shapes.

General::stop : Further output of Dot::dotsh will be suppressed during this calculation.

Transpose::nmtx : The first two levels of

$\{\{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538, \ll 12 \gg, 1.88462, 2.15385, 2.42308, 2.69231, 2.96154, 3.23077\}, \text{Abs}[\{\ll 1 \gg\}.\{\ll 1 \gg\}]\}$ cannot be transposed.

ListPlot::lpln :

Transpose[$\{\{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538, \ll 12 \gg, 1.88462, 2.15385, 2.42308, 2.69231, 2.96154, 3.23077\}, \text{Abs}[\ll 1 \gg]\}$] is not a list of numbers or pairs of numbers.

Transpose::nmtx : The first two levels of

$\{\{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538, \ll 12 \gg, 1.88462, 2.15385, 2.42308, 2.69231, 2.96154, 3.23077\}, \text{Abs}[\{\ll 1 \gg\}.\{\ll 1 \gg\}]\}$ cannot be transposed.

ListPlot::lpln :

Transpose[$\{\{-3.23077, -2.96154, -2.69231, -2.42308, -2.15385, -1.88462, -1.61538, \ll 12 \gg, 1.88462, 2.15385, 2.42308, 2.69231, 2.96154, 3.23077\}, \text{Abs}[\ll 1 \gg]\}$] is not a list of numbers or pairs of numbers.