Numerical matrix method for quantum periodic potentials

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Mathematica version...

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In[1]:= StringJoin[{"The running Mathematica version is ", ToString[$Version]}]
Out[1]= The running Mathematica version is 10.1.0  for Microsoft Windows (64-bit) (March 24, 2015)
```

Kronig - Penney model under an external field [$V_e(x)=\epsilon x$]

Functions that for a KP potential with lattice parameter a=1 and n_b barriers:
(I) evaluate the Hamiltonian matrix H^{KP}_{nm} [Eq. (17)] and H^{ϵ}_{nm} [Eq. (28)]
(II) solve Eq. (10) to find the eigenenergies and eigenfunctions. $\hbar\alpha$
The size of the system is $L=n_b*a=n_b$.
The positions of the nb barriers are stored in the vector (or list) xrV, and the corresponding widths and heights are stored in vectors bV and V0V, respectively.

Note that these vectors xrV, bV and V0V describe the periodic potential.
We use units such as $\hbar^2/2\mu=1$, μ being the mass of the particle.

Functions F_{nm} [Eq. (20)]

```
In[2]:= f[k_, x_, L_] := f[k, x, L] = Sin[k * Pi * x / L] / (Pi * k)
```

```
In[3]:= Fnm[n_, m_, x_, L_] := f[m - n, x, L] - f[m + n, x, L]
```

```
In[4]:= Fnn[n_, x_, L_] := x / L - f[2 * n, x, L]
```

Functions h_{nm} [Eq. (18)]

```
In[5]:= hnm[n_, m_, s_, b_, L_] := Fnm[n, m, s + b / 2, L] - Fnm[n, m, s - b / 2, L]
```

```
In[6]:= hnn[n_, s_, b_, L_] := Fnn[n, s + b / 2, L] - Fnn[n, s - b / 2, L]
```

Matrix elements H_{nm} [Eq. (17)]

In[7]:=
```
HHnn[n_, L_, V0V_, xrV_, bV_] := N[(n * Pi / L)^2 +
    Sum[V0V[[k]] * hnn[n, xrV[[k]], bV[[k]], L], {k, 1, Length[xrV]}] ]
```

In[8]:=
```
HHnm[n_, m_, L_, V0V_, xrV_, bV_] :=
 Sum[V0V[[k]] * hnm[n, m, xrV[[k]], bV[[k]], L], {k, 1, Length[xrV]}] // N
```

Matrix elements H^{ϵ}_{nm} corresponding to the external potential $V_e(x)=\epsilon x$=eps*x [Eq. (28)]

In[9]:=
```
HHnnε[eps_, L_] := N[eps * L / 2]
```

In[10]:=
```
HHnmε[n_, m_, eps_, L_] :=
 If[EvenQ[m + n], 0., N[-8 * m * n * eps * L / ((m^2 - n^2)^2 * Pi^2)]]
```

The function *HamiltonianMatrix* provides the $N \times N$ Hamiltonian matrix corresponding to the KP potential (given by xrV, bV and V0V) plus the external electric potential (defined by ϵ=eps). Here N=Nterms

In[11]:=
```
HamiltonianMatrix[Nterms_, L_, V0V_, xrV_, bV_, eps_] :=
 Table[If[n == m, HHnn[n, L, V0V, xrV, bV] + HHnnε[eps, L],
   HHnm[n, m, L, V0V, xrV, bV] + HHnmε[n, m, eps, L]],
  {n, 1, Nterms}, {m, 1, Nterms}]
```

The function *soluKPε* provides the solution of Eq. (13) for the KP model under a external field. The list of energies is provided directly by the function *EnV*. The n-th element of this matrix is the eigenvalue E_n
The matrix of coefficients $c_m^{(n)}$ of Eq. (14) are provided by *cnMatrix*. The element (n,m) of this matrix is just the coefficient $c_m^{(n)}$.

In[12]:=
```
soluKPε[Nterms_, L_, V0V_, xrV_, bV_, eps_] :=
 soluKPε[Nterms, L, V0V, xrV, bV, eps] =
  Eigensystem[N[HamiltonianMatrix[Nterms, L, V0V, xrV, bV, eps]]] // Chop //
     Transpose // Sort // Transpose
```

In[13]:=
```
EnV[Nterms_, L_, V0V_, xrV_, bV_, eps_] :=
 EnV[Nterms, L, V0V, xrV, bV, eps] = soluKPε[Nterms, L, V0V, xrV, bV, eps][[1]]
```

In[14]:=
```
cnMatrix[Nterms_, L_, V0V_, xrV_, bV_, eps_] :=
 cnMatrix[Nterms, L, V0V, xrV, bV, eps] =
  soluKPε[Nterms, L, V0V, xrV, bV, eps][[2]]
```

The function *psi* provides an estimate of n-th eigenfunction according the formula

$$\psi_n(x) \simeq \sum_{m=1}^{N^*} c_m^{(n)} \varphi_m(x)$$

When Nast=N^* is equal to Nterm=N, this expression is just Eq. (14).
The function ProbDensity is just $|\psi_n(x)|^2$

In[15]:=
```
psi[n_, x_, Nast_, Nterms_, L_, V0V_, xrV_, bV_, eps_] := Sqrt[2 / L] * Sum[
    cnMatrix[Nterms, L, V0V, xrV, bV, eps][[n, m]] * Sin[m * Pi * x / L], {m, 1, Nast}]
```

In[16]:=
```
ProbDensity[n_, x_, Nast_, Nterms_, L_, V0V_, xrV_, bV_, eps_] :=
 Abs[psi[n, x, Nast, Nterms, L, V0V, xrV, bV, eps]]^2
```

An example : n_b = 8, b = 1/4, V_0 =100, N=100

First, we generate the list of positions, widths and heights of the nb barriers of the KP potential

This is the case considered in Fig. 2: nb=8 barriers with width q=1/4 and height v0=100

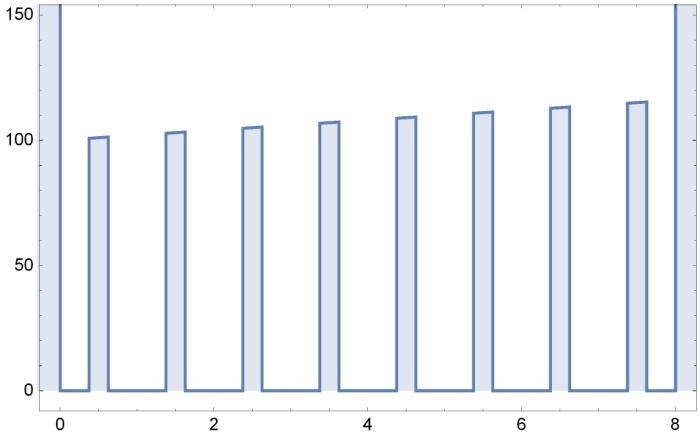
In[17]:=
```
nb = 8; L = N[nb]; v0 = 100.; q = 1. / 4;
{xrVector = Table[-1. / 2 + k, {k, 1, nb}], bVector = Table[q, {k, 1, nb}],
 V0Vector = Table[v0, {k, 1, nb}]}
```

Out[18]=
```
{{0.5, 1.5, 2.5, 3.5, 4.5, 5.5, 6.5, 7.5},
 {0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25, 0.25},
 {100., 100., 100., 100., 100., 100., 100., 100.}}
```

The next instruction generates a plot of the KP potential plus the external potential $V_e(x)=\epsilon x$ with ϵ=eps=2

In[19]:=
```
eps = 2;
leftWall = Plot[If[x < 0, 1.5 * v0 + eps * L, 0],
  {x, -1, 0.01}, Filling → Bottom, PlotPoints → 100, Frame → True];
rightWall = Plot[If[x > L, 1.5 * v0 + eps * L, 0], {x, L - 0.01, L + 1},
  Filling → Bottom, PlotPoints → 100, Frame → True];
KPpotential = KPpotential = Plot[Piecewise[Table[{eps * x + V0Vector[[k]],
      xrVector[[k]] - bVector[[k]] / 2 <= x <= xrVector[[k]] + bVector[[k]] / 2},
    {k, 1, nb}]], {x, 0, L}, Filling → Bottom, PlotPoints → 8000, Frame → True];
Show[leftWall, rightWall, KPpotential, PlotRange →
  {{-0.1, L + 0.1}, {0, 1.3 v0 + eps * L}}]
```

Out[20]=



Next one chooses the value of Nterm=N where N is the number of terms employed in the expansion of the sought eigenfunction [Eq. (12)]

In[21]:=
```
Nterms = 100;
```

The vector of the first N energies E_n is calculated by means of the function EnV

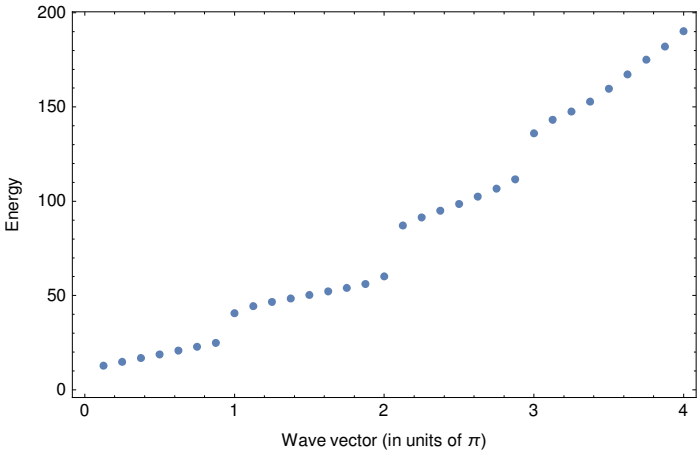
In[22]:=
```
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector, eps]
```

Out[22]=
```
{12.7254, 14.8143, 16.8165, 18.8169, 20.8167, 22.8176, 24.8854, 40.561, 44.3379,
 46.6254, 48.3999, 50.2903, 52.2179, 53.9672, 56.1516, 60.1351, 87.1121,
 91.4231, 94.9911, 98.6006, 102.516, 106.683, 111.638, 135.993, 143.223,
 147.571, 152.828, 159.662, 167.239, 175.066, 181.98, 190.187, 205.618, 215.397,
 225.444, 235.971, 246.907, 258.194, 269.693, 281.05, 294.123, 306.854,
 319.809, 333.065, 346.617, 360.435, 374.602, 393.74, 405.818, 420.177,
 435.501, 451.224, 467.293, 483.6, 499.768, 513.856, 535.434, 553.056, 570.971,
 589.225, 607.815, 626.723, 645.99, 666.862, 685.508, 705.577, 726.041,
 746.828, 768.171, 789.575, 811.316, 834.884, 855.807, 878.355, 901.29,
 924.533, 948.086, 971.929, 995.923, 1017.81, 1045.65, 1070.75, 1096.15,
 1121.88, 1149.09, 1175.43, 1202.08, 1231.51, 1256.55, 1284., 1311.86, 1340.05,
 1368.55, 1397.35, 1426.46, 1455.48, 1485.64, 1515.7, 1546.06, 1577.06}
```

Plot of the energies E_n obtained by means of the matrix method versus the wave number (in units of π)

In[23]:=
```
ListPlot[Table[{n / L, Energies[[n]]}, {n, 1, 4 * nb}], Frame → True,
 FrameLabel -> {"Wave vector (in units of π)", "Energy"}]
```

Out[23]=



Plot of the eigenfunctions

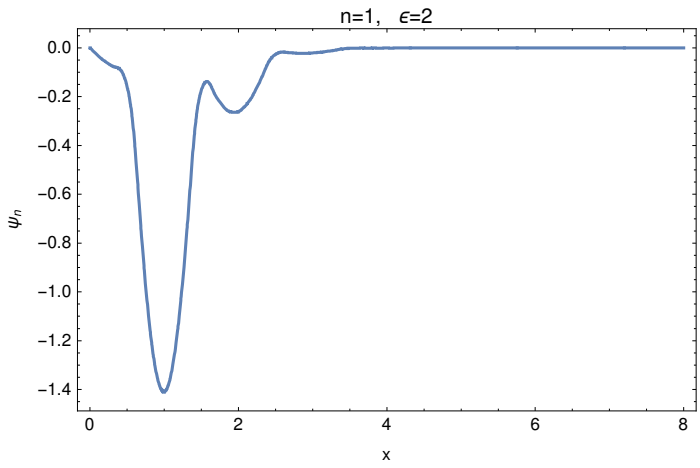
$$\psi_n(x) \simeq \sum_{m=1}^{N^*} c_m^{(n)} \varphi_m(x)$$

with Nast=N^* equal to Nterm=N .

Eigenfunction ψ_n(x) with n=nLevel=1

In[24]:=
```
nLevel = 1; Nast = Nterms;
Plot[-psi[nLevel, x, Nast, Nterms, L, V0Vector, xrVector, bVector, eps],
 {x, 0, L}, Frame → True, FrameLabel -> {"x", "ψn"},
 PlotLabel → StringJoin[{"n=", ToString[nLevel], ",    ϵ=", ToString[eps]}],
 PlotRange → All]
```

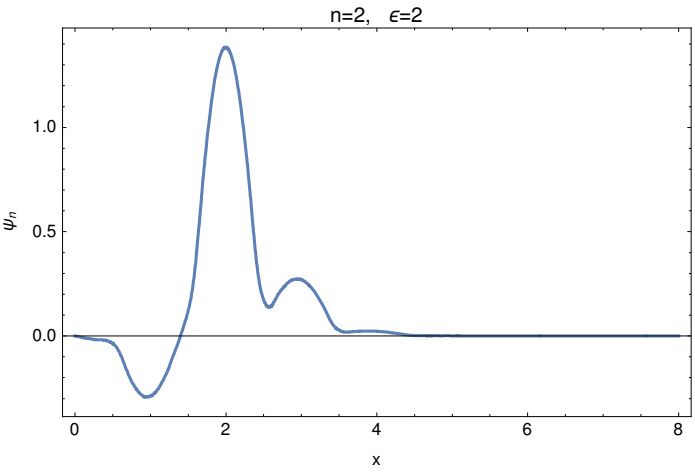
Out[24]=



Eigenfunction ψ_n(x) with n=nLevel=2

In[25]:=
```
nLevel = 2; Nast = Nterms;
Plot[-psi[nLevel, x, Nast, Nterms, L, V0Vector, xrVector, bVector, eps],
 {x, 0, L}, Frame → True, FrameLabel -> {"x", "ψn"},
 PlotLabel → StringJoin[{"n=", ToString[nLevel], ",    ϵ=", ToString[eps]}],
 PlotRange → All]
```

Out[25]=



Energies E_n for n_b = 20, b = 1/6, V_0 =100, N=100 and four external fields, ϵ=0,0.01, 0.5, 2 [cases of Fig. 10]

First, we define the KP potential: n_b = 20, b = 1/6, V_0 =100,

In[26]:=
```
nb = 20; L = N[nb]; v0 = 100.; q = 1. / 6;
{xrVector = Table[-1. / 2 + k, {k, 1, nb}], bVector = Table[q, {k, 1, nb}],
  V0Vector = Table[v0, {k, 1, nb}]};
```

First N energies E_n for ϵ=0 and N=100

In[28]:=
```
eps = 0;
Nterms = 100;
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector, eps];
EnExternalField[eps] = Table[{n / nb, Energies[[n]]}, {n, 1, Nterms}] // N
```

Out[31]=
```
{{0.05, 7.91235}, {0.1, 7.95139}, {0.15, 8.01592}, {0.2, 8.1051}, {0.25, 8.21774},
 {0.3, 8.35225}, {0.35, 8.50663}, {0.4, 8.67844}, {0.45, 8.86474}, {0.5, 9.06204},
 {0.55, 9.26632}, {0.6, 9.47297}, {0.65, 9.67686}, {0.7, 9.87238},
 {0.75, 10.0536}, {0.8, 10.2144}, {0.85, 10.349}, {0.9, 10.4522}, {0.95, 10.5198},
 {1., 30.9199}, {1.05, 31.5067}, {1.1, 31.6766}, {1.15, 31.9514}, {1.2, 32.3256},
 {1.25, 32.792}, {1.3, 33.3424}, {1.35, 33.967}, {1.4, 34.6557}, {1.45, 35.397},
 {1.5, 36.1787}, {1.55, 36.987}, {1.6, 37.8065}, {1.65, 38.6196}, {1.7, 39.4061},
 {1.75, 40.1425}, {1.8, 40.8027}, {1.85, 41.3585}, {1.9, 41.7816},
 {1.95, 42.0471}, {2., 42.1377}, {2.05, 69.5032}, {2.1, 69.919}, {2.15, 70.5925},
 {2.2, 71.4983}, {2.25, 72.6076}, {2.3, 73.8914}, {2.35, 75.3221},
 {2.4, 76.8745}, {2.45, 78.5255}, {2.5, 80.2532}, {2.55, 82.0362}, {2.6, 83.8517},
 {2.65, 85.6737}, {2.7, 87.4713}, {2.75, 89.205}, {2.8, 90.824}, {2.85, 92.2627},
 {2.9, 93.4407}, {2.95, 94.2698}, {3., 120.68}, {3.05, 123.881}, {3.1, 124.799},
 {3.15, 126.185}, {3.2, 127.952}, {3.25, 130.02}, {3.3, 132.324}, {3.35, 134.815},
 {3.4, 137.454}, {3.45, 140.212}, {3.5, 143.066}, {3.55, 145.993}, {3.6, 148.974},
 {3.65, 151.984}, {3.7, 154.996}, {3.75, 157.966}, {3.8, 160.831},
 {3.85, 163.483}, {3.9, 165.743}, {3.95, 167.329}, {4., 167.913}, {4.05, 191.449},
 {4.1, 193.216}, {4.15, 195.778}, {4.2, 198.854}, {4.25, 202.268}, {4.3, 205.913},
 {4.35, 209.73}, {4.4, 213.68}, {4.45, 217.74}, {4.5, 221.895}, {4.55, 226.133},
 {4.6, 230.448}, {4.65, 234.835}, {4.7, 239.288}, {4.75, 243.805},
 {4.8, 248.384}, {4.85, 253.024}, {4.9, 257.721}, {4.95, 262.476}, {5., 273.545}}
```

First N energies E_n for ϵ=0.01 and N=100

In[32]:=
```
eps = 0.01;
Nterms = 100;
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector, eps];
EnExternalField[eps] = Table[{n / nb, Energies[[n]]}, {n, 1, Nterms}] // N
```

Out[35]=
```
{{0.05, 7.98701}, {0.1, 8.05382}, {0.15, 8.12103}, {0.2, 8.20852}, {0.25, 8.31997},
 {0.3, 8.45376}, {0.35, 8.60769}, {0.4, 8.77918}, {0.45, 8.96523}, {0.5, 9.16232},
 {0.55, 9.36641}, {0.6, 9.57288}, {0.65, 9.77654}, {0.7, 9.97176},
 {0.75, 10.1525}, {0.8, 10.3127}, {0.85, 10.4462}, {0.9, 10.5497},
 {0.95, 10.6369}, {1., 31.0143}, {1.05, 31.6006}, {1.1, 31.7818}, {1.15, 32.0533},
 {1.2, 32.4266}, {1.25, 32.8926}, {1.3, 33.4427}, {1.35, 34.0673},
 {1.4, 34.7559}, {1.45, 35.4972}, {1.5, 36.2788}, {1.55, 37.087}, {1.6, 37.9065},
 {1.65, 38.7195}, {1.7, 39.5059}, {1.75, 40.2422}, {1.8, 40.9022},
 {1.85, 41.4574}, {1.9, 41.8781}, {1.95, 42.1261}, {2., 42.2664}, {2.05, 69.6001},
 {2.1, 70.0199}, {2.15, 70.693}, {2.2, 71.5985}, {2.25, 72.7078}, {2.3, 73.9915},
 {2.35, 75.4222}, {2.4, 76.9746}, {2.45, 78.6255}, {2.5, 80.3533},
 {2.55, 82.1363}, {2.6, 83.9517}, {2.65, 85.7737}, {2.7, 87.5713}, {2.75, 89.305},
 {2.8, 90.9239}, {2.85, 92.3625}, {2.9, 93.5404}, {2.95, 94.3714}, {3., 120.779},
 {3.05, 123.98}, {3.1, 124.899}, {3.15, 126.285}, {3.2, 128.052}, {3.25, 130.12},
 {3.3, 132.424}, {3.35, 134.915}, {3.4, 137.554}, {3.45, 140.312},
 {3.5, 143.166}, {3.55, 146.093}, {3.6, 149.074}, {3.65, 152.084},
 {3.7, 155.096}, {3.75, 158.066}, {3.8, 160.931}, {3.85, 163.583},
 {3.9, 165.842}, {3.95, 167.425}, {4., 168.018}, {4.05, 191.548}, {4.1, 193.317},
 {4.15, 195.878}, {4.2, 198.954}, {4.25, 202.368}, {4.3, 206.013},
 {4.35, 209.83}, {4.4, 213.78}, {4.45, 217.84}, {4.5, 221.995}, {4.55, 226.233},
 {4.6, 230.548}, {4.65, 234.935}, {4.7, 239.388}, {4.75, 243.905},
 {4.8, 248.484}, {4.85, 253.124}, {4.9, 257.821}, {4.95, 262.577}, {5., 273.646}}
```

First N energies E_n for ϵ=0.5 and N=100

In[36]:=
```
eps = 0.5;
Nterms = 100;
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector, eps];
EnExternalField[eps] = Table[{n / nb, Energies[[n]]}, {n, 1, Nterms}] // N
```

Out[39]=
```
{{0.05, 9.07104}, {0.1, 9.90626}, {0.15, 10.5586}, {0.2, 11.1177}, {0.25, 11.634},
 {0.3, 12.1371}, {0.35, 12.6376}, {0.4, 13.1377}, {0.45, 13.6378}, {0.5, 14.1378},
 {0.55, 14.6379}, {0.6, 15.1379}, {0.65, 15.6379}, {0.7, 16.1379},
 {0.75, 16.6384}, {0.8, 17.1444}, {0.85, 17.6852}, {0.9, 18.3323},
 {0.95, 19.2088}, {1., 32.1968}, {1.05, 34.0141}, {1.1, 35.2797}, {1.15, 36.3287},
 {1.2, 37.2599}, {1.25, 38.1029}, {1.3, 38.8813}, {1.35, 39.6022},
 {1.4, 40.2655}, {1.45, 40.8576}, {1.5, 41.4216}, {1.55, 42.0138},
 {1.6, 42.6031}, {1.65, 43.215}, {1.7, 43.9177}, {1.75, 44.7109}, {1.8, 45.5921},
 {1.85, 46.5801}, {1.9, 47.7166}, {1.95, 49.0974}, {2., 51.1448}, {2.05, 71.9622},
 {2.1, 73.8633}, {2.15, 75.3944}, {2.2, 76.7317}, {2.25, 77.9625},
 {2.3, 79.1988}, {2.35, 80.548}, {2.4, 82.0352}, {2.45, 83.6383}, {2.5, 85.3287},
 {2.55, 87.0791}, {2.6, 88.8619}, {2.65, 90.6465}, {2.7, 92.3963},
 {2.75, 94.0716}, {2.8, 95.6624}, {2.85, 97.2618}, {2.9, 99.0565},
 {2.95, 101.319}, {3., 123.729}, {3.05, 127.516}, {3.1, 129.95}, {3.15, 131.783},
 {3.2, 133.421}, {3.25, 135.279}, {3.3, 137.48}, {3.35, 139.918}, {3.4, 142.526},
 {3.45, 145.265}, {3.5, 148.103}, {3.55, 151.018}, {3.6, 153.986},
 {3.65, 156.981}, {3.7, 159.969}, {3.75, 162.895}, {3.8, 165.651},
 {3.85, 167.965}, {3.9, 169.84}, {3.95, 172.271}, {4., 176.041}, {4.05, 195.078},
 {4.1, 198.161}, {4.15, 200.922}, {4.2, 203.959}, {4.25, 207.335}, {4.3, 210.96},
 {4.35, 214.764}, {4.4, 218.707}, {4.45, 222.763}, {4.5, 226.914}, {4.55, 231.15},
 {4.6, 235.464}, {4.65, 239.849}, {4.7, 244.301}, {4.75, 248.818},
 {4.8, 253.396}, {4.85, 258.038}, {4.9, 262.758}, {4.95, 267.944}, {5., 278.925}}
```

First N energies E_n for ϵ=2 and N=100

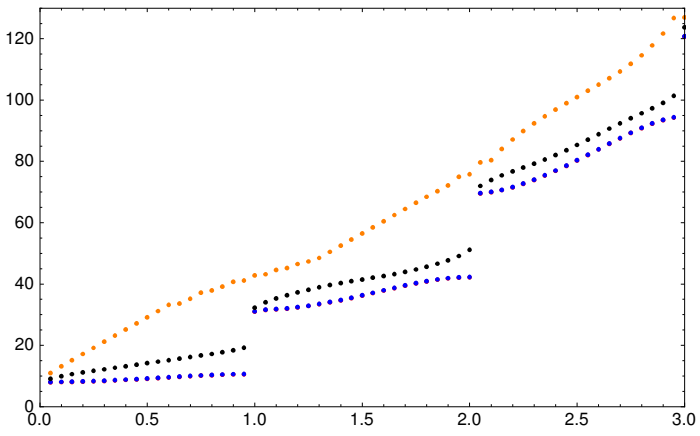
In[40]:=
```
eps = 2.;
Nterms = 100;
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector, eps];
EnExternalField[eps] = Table[{n / nb, Energies[[n]]}, {n, 1, Nterms}] // N
```

Out[43]=
```
{{0.05, 10.895}, {0.1, 13.1102}, {0.15, 15.1294}, {0.2, 17.1308}, {0.25, 19.1311},
 {0.3, 21.1313}, {0.35, 23.1313}, {0.4, 25.1314}, {0.45, 27.1314},
 {0.5, 29.1315}, {0.55, 31.1315}, {0.6, 33.1314}, {0.65, 33.5616},
 {0.7, 35.1316}, {0.75, 37.1315}, {0.8, 37.8638}, {0.85, 39.1316}, {0.9, 40.681},
 {0.95, 41.1315}, {1., 42.7864}, {1.05, 43.1315}, {1.1, 44.577}, {1.15, 45.1365},
 {1.2, 46.4725}, {1.25, 47.3043}, {1.3, 48.453}, {1.35, 50.4503}, {1.4, 52.4499},
 {1.45, 54.4497}, {1.5, 56.4495}, {1.55, 58.4493}, {1.6, 60.449}, {1.65, 62.4487},
 {1.7, 64.4481}, {1.75, 66.4439}, {1.8, 68.4023}, {1.85, 70.2064},
 {1.9, 72.1511}, {1.95, 74.9575}, {2., 75.8035}, {2.05, 79.6414}, {2.1, 80.3733},
 {2.15, 83.9866}, {2.2, 87.0898}, {2.25, 89.8533}, {2.3, 92.3655},
 {2.35, 94.6845}, {2.4, 96.8602}, {2.45, 98.9425}, {2.5, 100.976}, {2.55, 102.991},
 {2.6, 105.016}, {2.65, 107.097}, {2.7, 109.319}, {2.75, 111.777},
 {2.8, 114.561}, {2.85, 117.789}, {2.9, 121.674}, {2.95, 126.732}, {3., 126.923},
 {3.05, 134.44}, {3.1, 139.592}, {3.15, 143.784}, {3.2, 147.466}, {3.25, 150.779},
 {3.3, 153.822}, {3.35, 156.628}, {3.4, 159.194}, {3.45, 161.541},
 {3.5, 163.876}, {3.55, 166.337}, {3.6, 168.811}, {3.65, 171.26}, {3.7, 173.924},
 {3.75, 176.966}, {3.8, 180.401}, {3.85, 184.297}, {3.9, 188.839},
 {3.95, 194.476}, {4., 201.205}, {4.05, 203.142}, {4.1, 208.233}, {4.15, 213.698},
 {4.2, 218.362}, {4.25, 222.535}, {4.3, 226.429}, {4.35, 230.245},
 {4.4, 234.123}, {4.45, 238.113}, {4.5, 242.214}, {4.55, 246.414},
 {4.6, 250.702}, {4.65, 255.072}, {4.7, 259.526}, {4.75, 264.089},
 {4.8, 268.85}, {4.85, 274.023}, {4.9, 280.008}, {4.95, 287.673}, {5., 299.042}}
```

Plot of E_n versus the wave number (in units of π) for ϵ=0,0.01, 0.5, 1 (red, blue, black, orange and green points, respectively)

In[44]:=
```
ListPlot[{EnExternalField[0], EnExternalField[0.01],
  EnExternalField[0.5], EnExternalField[2.]}, PlotRange → {{0, 3}, {0, 130}},
 PlotStyle → {Red, Blue, Black, Orange, Green}, Frame → True]
```

Out[44]=



First eigenfunction ψ_1 for n_b = 20, b = 1/6, V_0 =100, N=100 and four external fields, ϵ=0,0.01, 0.5, 2 [cases of Fig. 11]

First, we define the KP potential: n_b = 20, b = 1/6, V_0 =100,

In[45]:=
```
nb = 20; L = N[nb]; v0 = 100.; q = 1. / 6;
{xrVector = Table[-1. / 2 + k, {k, 1, nb}], bVector = Table[q, {k, 1, nb}],
  V0Vector = Table[v0, {k, 1, nb}]};
```

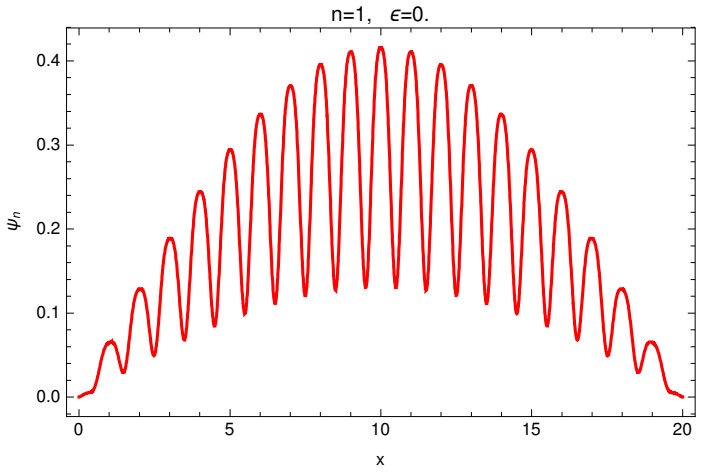
Next one chooses the value of Nterm=*N*

In[47]:=
```
Nterms = 100;
```

Eigenfunction ψ_1(x) for ϵ=0

In[48]:=
```
eps = 0.;
nLevel = 1;
Nast = Nterms;
PsinExternalField[eps] =
 Plot[psi[nLevel, x, Nast, Nterms, L, V0Vector, xrVector, bVector, eps], {x, 0, L},
  PlotRange → All, Frame → True, FrameLabel -> {"x", "ψn"}, PlotLabel → StringJoin[
    {"n=", ToString[nLevel], ",    ϵ=", ToString[eps]}], PlotStyle → Red]
```

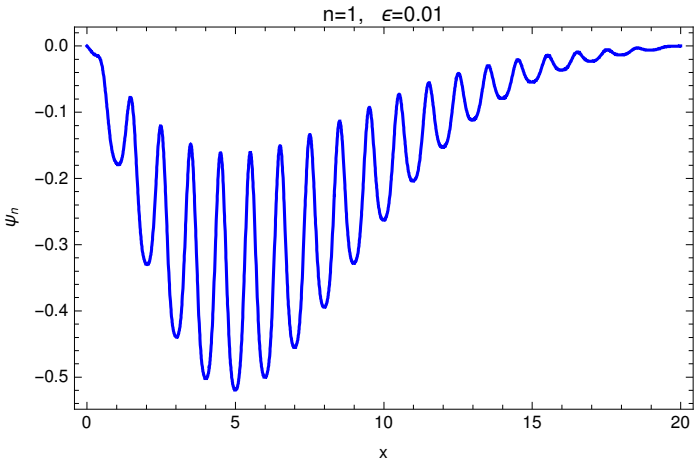
Out[50]=



Eigenfunction ψ_1(x) for ϵ=0.01

In[51]:=
```
eps = 0.01;
nLevel = 1;
Nast = Nterms;
PsinExternalField[eps] = Plot[
  -psi[nLevel, x, Nast, Nterms, L, V0Vector, xrVector, bVector, eps], {x, 0, L},
  PlotRange → All, Frame → True, FrameLabel -> {"x", "ψn"}, PlotLabel → StringJoin[
    {"n=", ToString[nLevel], ",    ϵ=", ToString[eps]}], PlotStyle → Blue]
```

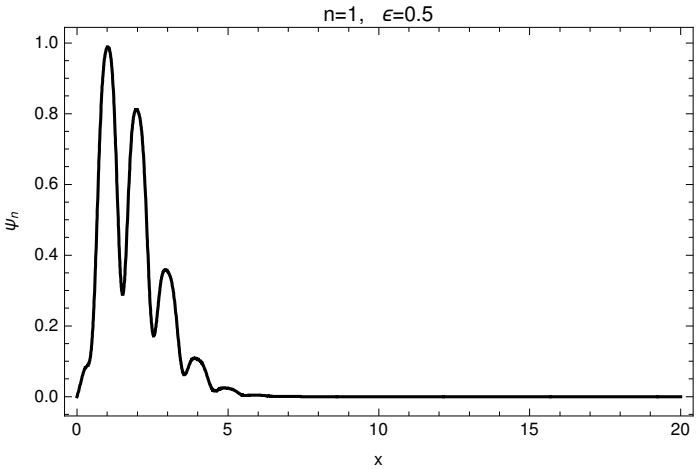
Out[52]=



Eigenfunction $\psi_1(x)$ for ϵ=0.5

In[53]:=
```
eps = 0.5;
nLevel = 1;
Nast = Nterms;
PsinExternalField[eps] = Plot[
  -psi[nLevel, x, Nast, Nterms, L, V0Vector, xrVector, bVector, eps], {x, 0, L},
  PlotRange → All, Frame → True, FrameLabel -> {"x", "ψn"}, PlotLabel → StringJoin[
    {"n=", ToString[nLevel], ",    ϵ=", ToString[eps]}], PlotStyle → Black]
```

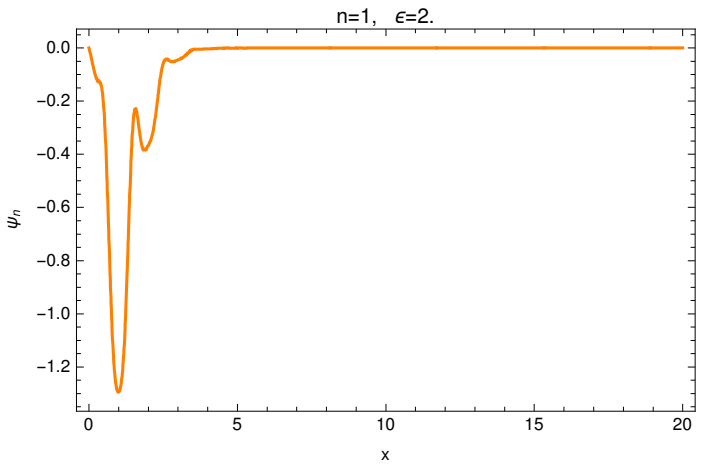
Out[54]=



Eigenfunction $\psi_1(x)$ for ϵ=2

In[55]:=
```
eps = 2.;
nLevel = 1;
Nast = Nterms;
PsinExternalField[eps] =
 Plot[psi[nLevel, x, Nast, Nterms, L, V0Vector, xrVector, bVector, eps], {x, 0, L},
  PlotRange → All, Frame → True, FrameLabel -> {"x", "ψn"}, PlotLabel → StringJoin[
    {"n=", ToString[nLevel], ",    ϵ=", ToString[eps]}], PlotStyle → Orange]
```

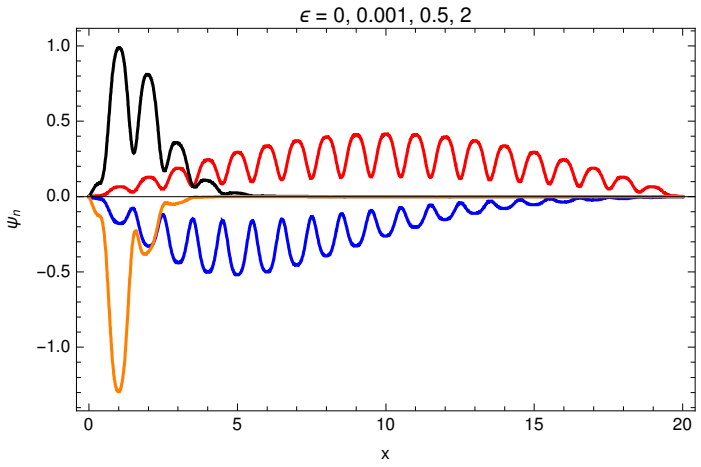
Out[56]=



Plot of $\psi_1(x)$ for $\epsilon = 0, 0.001, 0.5, 2$ (red, blue, black and orange lines, respectively)

In[57]:=
```
Show[{PsinExternalField[0.], PsinExternalField[0.01],
  PsinExternalField[0.5], PsinExternalField[2.]},
 PlotRange → All, PlotLabel → StringJoin[{ "ϵ = 0, 0.001, 0.5, 2"}]]
```

Out[57]=



Time evolution of quantum states

Mathematica instructions to evaluate the time evolution of a Gaussian wave packet

The quantum state at time zero is the Gaussian wave packet

$$\Psi(x,0) = \frac{1}{(\pi\sigma^2)^{1/4}} \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]$$

Here $x_0 \equiv$ x0 and $\sigma^2 \equiv$ sig2

In[58]:=
```
psiGaussiana[x_, x0_, sig2_] := 1 / (Pi * sig2) ^ (1 / 4) * Exp[- (x - x0) ^2 / (2 * sig2)]
```

The function *dcoef* gives the coefficients $\langle\varphi_m|\Psi(x,0)\rangle$ of Eq. (30) and (31)

In[59]:=
```
dcoef[m_, x0_, sig2_, L_] :=
 dcoef[m, x0, sig2, L] = If[OddQ[m], Sqrt[2 / L] * NIntegrate[
       Sin[m * Pi * x / L] * psiGaussiana[x, x0, sig2], {x, 0, L}], 0] // Chop
```

The function *acoef* gives the coefficients $a_n = \langle\psi_n|\Psi(x,0)\rangle$ of Eq. (30)

In[60]:=
```
acoef[n_, x0_, sig2_, L_, Nterms_, V0V_, xrV_, bV_, eps_] :=
 acoef[n, x0, sig2, L, Nterms, V0V, xrV, bV, eps] =
  Sum[cnMatrix[Nterms, L, V0V, xrV, bV, eps][[n, m]] *
    dcoef[m, x0, sig2, L], {m, 1, Nterms}]
```

The function *PsiXT* evaluate the wave function $\Psi(x,t)$ by means of the expression

$$\Psi(x,t) \approx \sum_{n=1}^{N} a_n\, e^{-iE_n t/\hbar}\, \psi_n(x)$$ [see Eq. (29]

We use units such as $\hbar = 1$

In[61]:=
```
PsiXT[x_, t_, x0_, sig2_, L_, Nterms_, V0V_, xrV_, bV_, eps_] :=
 (Energies = EnV[Nterms, L, V0V, xrV, bV, eps];
  Sum[acoef[n, x0, sig2, L, Nterms, V0V, xrV, bV, eps] * psi[n, x, Nterms, Nterms,
     L, V0V, xrV, bV, eps] * Exp[-I * Energies[[n]] * t], {n, 1, Nterms}])
```

$|\Psi(x,t)|^2$ is given by the function *ProbDensityXT*

In[62]:=
```
ProbDensityXT[x_, t_, x0_, sig2_, L_, Nterms_, V0V_, xrV_, bV_, eps_] :=
 Abs[PsiXT[x, t, x0, sig2, L, Nterms, V0V, xrV, bV, eps]]^2
```

In[63]:=

Example of Fig. 12: we evaluate $|\Psi(x,t{=}0.26)|^2$ for an initial Gaussian wave packet with $x_0 = L/2$ and $\sigma^2 \equiv 0.05$ inside the KP potential with n_b=L = 10, b = 1/6, and:

- Case 1: V_0 =5 and ϵ=0
- Case 2: V_0 =5 and ϵ=0

● Case 3: V_0 =0 and ϵ=10

In all cases N=100

In[64]:=
```
nb = 10; L = N[nb]; q = 1. / 6;
x0 = L / 2.; sig2 = 0.05;
{xrVector = Table[-1. / 2 + k, {k, 1, nb}], bVector = Table[q, {k, 1, nb}]};
Nterms = 100;
```

Case 1: V_0 =0 and ϵ=0.

We save in *denProb* a table of values {x, $|\Psi(x,t=0.26)|^2$} for x=0,L/200,2L/200,...,L

In[68]:=
```
With[{t = 0.26, v0 = 0., eps = 0.},
 V0Vector = Table[v0, {k, 1, nb}];
 denProb[t, v0, eps] = Table[{x, ProbDensityXT[x, t, x0, sig2, L,
       Nterms, V0Vector, xrVector, bVector, eps]} // N, {x, 0, L, L/200}]]
```

Out[68]=
```
{{0., 0.}, {0.05, 0.00210186}, {0.1, 0.00664813}, {0.15, 0.0098517},
 {0.2, 0.00910271}, {0.25, 0.0051662}, {0.3, 0.0015159}, {0.35, 0.00138597},
 {0.4, 0.00505171}, {0.45, 0.00963367}, {0.5, 0.0115607}, {0.55, 0.0095795},
 {0.6, 0.00576668}, {0.65, 0.00372674}, {0.7, 0.00554364}, {0.75, 0.0100733},
 {0.8, 0.0139796}, {0.85, 0.014579}, {0.9, 0.0120622}, {0.95, 0.00925176},
 {1., 0.00917031}, {1.05, 0.0125205}, {1.1, 0.017184}, {1.15, 0.0200862},
 {1.2, 0.0197865}, {1.25, 0.0176089}, {1.3, 0.0164307}, {1.35, 0.018235},
 {1.4, 0.0225131}, {1.45, 0.0268045}, {1.5, 0.0288255}, {1.55, 0.0283459},
 {1.6, 0.0272727}, {1.65, 0.0279656}, {1.7, 0.031272}, {1.75, 0.0359188},
 {1.8, 0.0396857}, {1.85, 0.0412861}, {1.9, 0.041365}, {1.95, 0.0418467},
 {2., 0.0442763}, {2.05, 0.0485819}, {2.1, 0.0532469}, {2.15, 0.0566516},
 {2.2, 0.0584025}, {2.25, 0.0595611}, {2.3, 0.0616686}, {2.35, 0.065453},
 {2.4, 0.0703019}, {2.45, 0.0748678}, {2.5, 0.0782221}, {2.55, 0.0805714},
 {2.6, 0.0829899}, {2.65, 0.0864711}, {2.7, 0.091129}, {2.75, 0.0961834},
 {2.8, 0.100671}, {2.85, 0.104236}, {2.9, 0.107357}, {2.95, 0.110873},
 {3., 0.11527}, {3.05, 0.12032}, {3.1, 0.125334}, {3.15, 0.129758},
 {3.2, 0.133599}, {3.25, 0.137352}, {3.3, 0.141545}, {3.35, 0.146307},
 {3.4, 0.151302}, {3.45, 0.156047}, {3.5, 0.160306}, {3.55, 0.164244},
 {3.6, 0.168239}, {3.65, 0.172548}, {3.7, 0.177112}, {3.75, 0.181634},
 {3.8, 0.185839}, {3.85, 0.18968}, {3.9, 0.19334}, {3.95, 0.197047},
 {4., 0.200883}, {4.05, 0.204732}, {4.1, 0.20839}, {4.15, 0.211735}, {4.2, 0.2148},
 {4.25, 0.217719}, {4.3, 0.2206}, {4.35, 0.223442}, {4.4, 0.226144},
 {4.45, 0.228598}, {4.5, 0.230765}, {4.55, 0.232687}, {4.6, 0.234438},
 {4.65, 0.236056}, {4.7, 0.237522}, {4.75, 0.238783}, {4.8, 0.239796},
 {4.85, 0.240547}, {4.9, 0.241056}, {4.95, 0.241347}, {5., 0.241442},
 {5.05, 0.241347}, {5.1, 0.241056}, {5.15, 0.240547}, {5.2, 0.239796},
 {5.25, 0.238783}, {5.3, 0.237522}, {5.35, 0.236056}, {5.4, 0.234438},
 {5.45, 0.232687}, {5.5, 0.230765}, {5.55, 0.228598}, {5.6, 0.226144},
 {5.65, 0.223442}, {5.7, 0.2206}, {5.75, 0.217719}, {5.8, 0.2148},
 {5.85, 0.211735}, {5.9, 0.20839}, {5.95, 0.204732}, {6., 0.200883},
```

```
{6.05, 0.197047}, {6.1, 0.19334}, {6.15, 0.18968}, {6.2, 0.185839},
{6.25, 0.181634}, {6.3, 0.177112}, {6.35, 0.172548}, {6.4, 0.168239},
{6.45, 0.164244}, {6.5, 0.160306}, {6.55, 0.156047}, {6.6, 0.151302},
{6.65, 0.146307}, {6.7, 0.141545}, {6.75, 0.137352}, {6.8, 0.133599},
{6.85, 0.129758}, {6.9, 0.125334}, {6.95, 0.12032}, {7., 0.11527},
{7.05, 0.110873}, {7.1, 0.107357}, {7.15, 0.104236}, {7.2, 0.100671},
{7.25, 0.0961834}, {7.3, 0.091129}, {7.35, 0.0864711}, {7.4, 0.0829899},
{7.45, 0.0805714}, {7.5, 0.0782221}, {7.55, 0.0748678}, {7.6, 0.0703019},
{7.65, 0.065453}, {7.7, 0.0616686}, {7.75, 0.0595611}, {7.8, 0.0584025},
{7.85, 0.0566516}, {7.9, 0.0532469}, {7.95, 0.0485819}, {8., 0.0442763},
{8.05, 0.0418467}, {8.1, 0.041365}, {8.15, 0.0412861}, {8.2, 0.0396857},
{8.25, 0.0359188}, {8.3, 0.031272}, {8.35, 0.0279656}, {8.4, 0.0272727},
{8.45, 0.0283459}, {8.5, 0.0288255}, {8.55, 0.0268045}, {8.6, 0.0225131},
{8.65, 0.018235}, {8.7, 0.0164307}, {8.75, 0.0176089}, {8.8, 0.0197865},
{8.85, 0.0200862}, {8.9, 0.017184}, {8.95, 0.0125205}, {9., 0.00917031},
{9.05, 0.00925176}, {9.1, 0.0120622}, {9.15, 0.014579}, {9.2, 0.0139796},
{9.25, 0.0100733}, {9.3, 0.00554364}, {9.35, 0.00372674}, {9.4, 0.00576668},
{9.45, 0.0095795}, {9.5, 0.0115607}, {9.55, 0.00963367}, {9.6, 0.00505171},
{9.65, 0.00138597}, {9.7, 0.0015159}, {9.75, 0.0051662}, {9.8, 0.00910271},
{9.85, 0.0098517}, {9.9, 0.00664813}, {9.95, 0.00210186}, {10., 2.4647×10^-32}}
```

Case 2: V_0 =5 and ϵ=0

We save in *denProb* a table of values {x, $|\Psi(x,t{=}0.26)|^2$} for x=0,L/200,2L/200,...,L

In[69]:=
```
With[{t = 0.26, v0 = 5., eps = 0.},
 V0Vector = Table[v0, {k, 1, nb}];
 denProb[t, v0, eps] = Table[{x, ProbDensityXT[x, t, x0, sig2, L,
      Nterms, V0Vector, xrVector, bVector, eps]} // N, {x, 0, L, L/200}]]
```

Out[69]=
```
{{0., 0.}, {0.05, 0.00200875}, {0.1, 0.00631217}, {0.15, 0.0092872},
 {0.2, 0.00851593}, {0.25, 0.00475663}, {0.3, 0.00133636},
 {0.35, 0.00133553}, {0.4, 0.00489542}, {0.45, 0.00922949},
 {0.5, 0.011124}, {0.55, 0.00944628}, {0.6, 0.00590403}, {0.65, 0.00373266},
 {0.7, 0.00508065}, {0.75, 0.00914309}, {0.8, 0.0128768}, {0.85, 0.0136733},
 {0.9, 0.0115379}, {0.95, 0.00899671}, {1., 0.00889976}, {1.05, 0.0119702},
 {1.1, 0.0162447}, {1.15, 0.018871}, {1.2, 0.0185593}, {1.25, 0.016598},
 {1.3, 0.0156884}, {1.35, 0.0175856}, {1.4, 0.0216533}, {1.45, 0.0256799},
 {1.5, 0.0279126}, {1.55, 0.0282842}, {1.6, 0.0281448}, {1.65, 0.0290536},
 {1.7, 0.0315011}, {1.75, 0.0345085}, {1.8, 0.036537}, {1.85, 0.0369838},
 {1.9, 0.0368968}, {1.95, 0.0381382}, {2., 0.0416915}, {2.05, 0.0467027},
 {2.1, 0.0511039}, {2.15, 0.053219}, {2.2, 0.0530775}, {2.25, 0.0524069},
 {2.3, 0.0532361}, {2.35, 0.0563078}, {2.4, 0.0608212}, {2.45, 0.0656291},
 {2.5, 0.0703592}, {2.55, 0.0752743}, {2.6, 0.08042}, {2.65, 0.085217},
 {2.7, 0.0888035}, {2.75, 0.0905675}, {2.8, 0.0904178}, {2.85, 0.0889252},
 {2.9, 0.0873735}, {2.95, 0.0873057}, {3., 0.0896248}, {3.05, 0.0941053},
 {3.1, 0.0997574}, {3.15, 0.10556}, {3.2, 0.110982}, {3.25, 0.116028},
 {3.3, 0.120764}, {3.35, 0.124841}, {3.4, 0.127923}, {3.45, 0.130767},
```

```
{3.5, 0.135277}, {3.55, 0.143006}, {3.6, 0.153813}, {3.65, 0.166225},
{3.7, 0.17876}, {3.75, 0.190484}, {3.8, 0.200612}, {3.85, 0.208317},
{3.9, 0.213045}, {3.95, 0.214691}, {4., 0.213489}, {4.05, 0.209931},
{4.1, 0.20469}, {4.15, 0.198567}, {4.2, 0.192632}, {4.25, 0.188173},
{4.3, 0.186059}, {4.35, 0.186262}, {4.4, 0.188662}, {4.45, 0.194316},
{4.5, 0.205203}, {4.55, 0.222272}, {4.6, 0.244048}, {4.65, 0.267423},
{4.7, 0.289738}, {4.75, 0.309804}, {4.8, 0.327168}, {4.85, 0.341217},
{4.9, 0.351289}, {4.95, 0.357172}, {5., 0.35908}, {5.05, 0.357172},
{5.1, 0.351289}, {5.15, 0.341217}, {5.2, 0.327168}, {5.25, 0.309804},
{5.3, 0.289738}, {5.35, 0.267423}, {5.4, 0.244048}, {5.45, 0.222272},
{5.5, 0.205203}, {5.55, 0.194316}, {5.6, 0.188662}, {5.65, 0.186262},
{5.7, 0.186059}, {5.75, 0.188173}, {5.8, 0.192632}, {5.85, 0.198567},
{5.9, 0.20469}, {5.95, 0.209931}, {6., 0.213489}, {6.05, 0.214691},
{6.1, 0.213045}, {6.15, 0.208317}, {6.2, 0.200612}, {6.25, 0.190484},
{6.3, 0.17876}, {6.35, 0.166225}, {6.4, 0.153813}, {6.45, 0.143006},
{6.5, 0.135277}, {6.55, 0.130767}, {6.6, 0.127923}, {6.65, 0.124841},
{6.7, 0.120764}, {6.75, 0.116028}, {6.8, 0.110982}, {6.85, 0.10556},
{6.9, 0.0997574}, {6.95, 0.0941053}, {7., 0.0896248}, {7.05, 0.0873057},
{7.1, 0.0873735}, {7.15, 0.0889252}, {7.2, 0.0904178}, {7.25, 0.0905675},
{7.3, 0.0888035}, {7.35, 0.085217}, {7.4, 0.08042}, {7.45, 0.0752743},
{7.5, 0.0703592}, {7.55, 0.0656291}, {7.6, 0.0608212}, {7.65, 0.0563078},
{7.7, 0.0532361}, {7.75, 0.0524069}, {7.8, 0.0530775}, {7.85, 0.053219},
{7.9, 0.0511039}, {7.95, 0.0467027}, {8., 0.0416915}, {8.05, 0.0381382},
{8.1, 0.0368968}, {8.15, 0.0369838}, {8.2, 0.036537}, {8.25, 0.0345085},
{8.3, 0.0315011}, {8.35, 0.0290536}, {8.4, 0.0281448}, {8.45, 0.0282842},
{8.5, 0.0279126}, {8.55, 0.0256799}, {8.6, 0.0216533}, {8.65, 0.0175856},
{8.7, 0.0156884}, {8.75, 0.016598}, {8.8, 0.0185593}, {8.85, 0.018871},
{8.9, 0.0162447}, {8.95, 0.0119702}, {9., 0.00889976}, {9.05, 0.00899671},
{9.1, 0.0115379}, {9.15, 0.0136733}, {9.2, 0.0128768}, {9.25, 0.00914309},
{9.3, 0.00508065}, {9.35, 0.00373266}, {9.4, 0.00590403}, {9.45, 0.00944628},
{9.5, 0.011124}, {9.55, 0.00922949}, {9.6, 0.00489542}, {9.65, 0.00133553},
{9.7, 0.00133636}, {9.75, 0.00475663}, {9.8, 0.00851593}, {9.85, 0.0092872},
{9.9, 0.00631217}, {9.95, 0.00200875}, {10., 2.20575 × 10^-32}}
```

Case 3: V_0 =0 and ϵ=10

We save in *denProb* a table of values {x, $|\Psi(x,t{=}0.26)|^2$} for x=0,L/200,2L/200,...,L

In[70]:=
```
With[{t = 0.26, v0 = 0., eps = 10.},
 V0Vector = Table[v0, {k, 1, nb}];
 denProb[t, v0, eps] = Table[{x, ProbDensityXT[x, t, x0, sig2, L,
      Nterms, V0Vector, xrVector, bVector, eps]} // N, {x, 0, L, L/200}]]
```

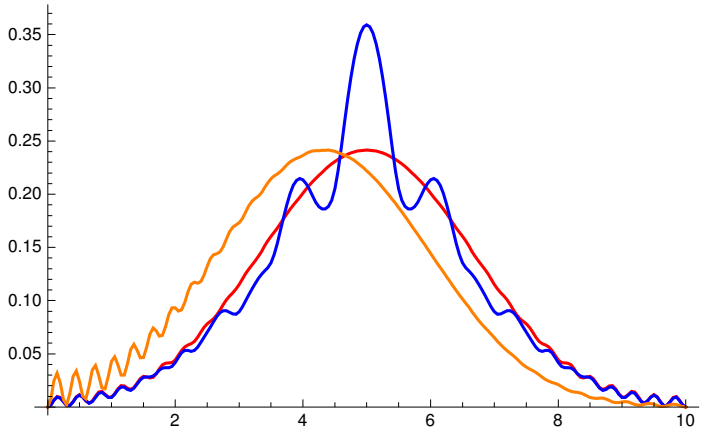
Out[70]=
```
{{0., 0.}, {0.05, 0.00839788}, {0.1, 0.0247109}, {0.15, 0.0318061},
 {0.2, 0.0225129}, {0.25, 0.0070335}, {0.3, 0.00197952}, {0.35, 0.0129499},
 {0.4, 0.028936}, {0.45, 0.0340571}, {0.5, 0.0240225}, {0.55, 0.0102272},
 {0.6, 0.00768835}, {0.65, 0.0196852}, {0.7, 0.0348146}, {0.75, 0.0389807},
 {0.8, 0.0296455}, {0.85, 0.017929}, {0.9, 0.0169882}, {0.95, 0.0288797},
```

{1., 0.0430122}, {1.05, 0.0471574}, {1.1, 0.039533}, {1.15, 0.0300282},
{1.2, 0.0299635}, {1.25, 0.0410216}, {1.3, 0.0541528}, {1.35, 0.0589187},
{1.4, 0.0536131}, {1.45, 0.0463646}, {1.5, 0.0467502}, {1.55, 0.0565807},
{1.6, 0.0686993}, {1.65, 0.0743685}, {1.7, 0.0716261}, {1.75, 0.0666418},
{1.8, 0.0673245}, {1.85, 0.0757891}, {1.9, 0.0868331}, {1.95, 0.093355},
{2., 0.0930932}, {2.05, 0.0903139}, {2.1, 0.0913174}, {2.15, 0.0984583},
{2.2, 0.108331}, {2.25, 0.115402}, {2.3, 0.117257}, {2.35, 0.116498},
{2.4, 0.1179}, {2.45, 0.123861}, {2.5, 0.132464}, {2.55, 0.139637},
{2.6, 0.143031}, {2.65, 0.143945}, {2.7, 0.145765}, {2.75, 0.150711},
{2.8, 0.157969}, {2.85, 0.164754}, {2.9, 0.16899}, {2.95, 0.171069},
{3., 0.173201}, {3.05, 0.177249}, {3.1, 0.183116}, {3.15, 0.189064},
{3.2, 0.193428}, {3.25, 0.19606}, {3.3, 0.198258}, {3.35, 0.201439},
{3.4, 0.205886}, {3.45, 0.21064}, {3.5, 0.214492}, {3.55, 0.217052},
{3.6, 0.218972}, {3.65, 0.221229}, {3.7, 0.224234}, {3.75, 0.227555},
{3.8, 0.230397}, {3.85, 0.232335}, {3.9, 0.233612}, {3.95, 0.234833},
{4., 0.23639}, {4.05, 0.238157}, {4.1, 0.239674}, {4.15, 0.240584},
{4.2, 0.240915}, {4.25, 0.240995}, {4.3, 0.241127}, {4.35, 0.241336},
{4.4, 0.241396}, {4.45, 0.241058}, {4.5, 0.240266}, {4.55, 0.239166},
{4.6, 0.237954}, {4.65, 0.236708}, {4.7, 0.235346}, {4.75, 0.23373},
{4.8, 0.231788}, {4.85, 0.229567}, {4.9, 0.227173}, {4.95, 0.224677},
{5., 0.222072}, {5.05, 0.219301}, {5.1, 0.216325}, {5.15, 0.213149},
{5.2, 0.209815}, {5.25, 0.206361}, {5.3, 0.202798}, {5.35, 0.199122},
{5.4, 0.195331}, {5.45, 0.191438}, {5.5, 0.187458}, {5.55, 0.183392},
{5.6, 0.179233}, {5.65, 0.17498}, {5.7, 0.170663}, {5.75, 0.166324},
{5.8, 0.161994}, {5.85, 0.157663}, {5.9, 0.153289}, {5.95, 0.148838},
{6., 0.144326}, {6.05, 0.139818}, {6.1, 0.13539}, {6.15, 0.131072},
{6.2, 0.126814}, {6.25, 0.122535}, {6.3, 0.118182}, {6.35, 0.113794},
{6.4, 0.109478}, {6.45, 0.105342}, {6.5, 0.101402}, {6.55, 0.0975653},
{6.6, 0.0937002}, {6.65, 0.0897408}, {6.7, 0.0857538}, {6.75, 0.0819001},
{6.8, 0.0783171}, {6.85, 0.0750074}, {6.9, 0.0718244}, {6.95, 0.0685781},
{7., 0.0651857}, {7.05, 0.0617499}, {7.1, 0.0584949}, {7.15, 0.0555988},
{7.2, 0.0530479}, {7.25, 0.050631}, {7.3, 0.0480904}, {7.35, 0.0453219},
{7.4, 0.0424695}, {7.45, 0.0398316}, {7.5, 0.0376373}, {7.55, 0.0358608},
{7.6, 0.0342211}, {7.65, 0.0323818}, {7.7, 0.0302081}, {7.75, 0.0278841},
{7.8, 0.0257901}, {7.85, 0.0242199}, {7.9, 0.023147}, {7.95, 0.022224},
{8., 0.0210275}, {8.05, 0.0193758}, {8.1, 0.0174795}, {8.15, 0.0158004},
{8.2, 0.0147127}, {8.25, 0.0142142}, {8.3, 0.0139073}, {8.35, 0.0132778},
{8.4, 0.0120728}, {8.45, 0.0104991}, {8.5, 0.00908634}, {8.55, 0.00830482},
{8.6, 0.00821391}, {8.65, 0.00840201}, {8.7, 0.0082712}, {8.75, 0.00746741},
{8.8, 0.00614452}, {8.85, 0.00486526}, {8.9, 0.00420327},
{8.95, 0.00432824}, {9., 0.00487338}, {9.05, 0.00518542}, {9.1, 0.00478368},
{9.15, 0.00370312}, {9.2, 0.00247648}, {9.25, 0.00176528}, {9.3, 0.00189691},
{9.35, 0.00263188}, {9.4, 0.00332459}, {9.45, 0.00336598}, {9.5, 0.00260161},
{9.55, 0.00143825}, {9.6, 0.000567436}, {9.65, 0.000496605},
{9.7, 0.00120748}, {9.75, 0.00217009}, {9.8, 0.0026976}, {9.85, 0.00240159},
{9.9, 0.00144499}, {9.95, 0.000429465}, $\{10., 1.07623 \times 10^{-30}\}\}$

Plot of $|\Psi(x,t{=}0.26)|^2$ for Case 1, 2 and 3 (red, blue and orange lines)
We save in *denProb* a table of values {x, $|\Psi(x,t{=}0.26)|^2$} for x=0,L/200,2L/200,...,L

In[71]:=
```
ListPlot[{denProb[0.26, 0., 0.], denProb[0.26, 5., 0.], denProb[0.26, 0., 10.]},
 Joined → True, PlotStyle → {Red, Blue, Orange}]
```

Out[71]=



In[72]:=

An additional task: position of the wave packet and comparison with Newton's second law

xMaxt[t,v0,eps,np] provides the position x_{max} of the maximum value $|\Psi(x_{max},t)|^2$ of the wave packet $|\Psi(x,t)|^2$ for x=0,Δ,2Δ,...L with Δ=L/np
The values of x_0, σ^2≡, n_b=L, b of the case one wants to solve must be defined before using xMaxt

In[73]:=
```
xProbMax[xPsiVector_] :=
 xPsiVector[[Position[xPsiVector, Max[Transpose[xPsiVector][[2]]]][[1, 1]]]]
```

In[74]:=
```
xMaxt[t_, v0_, eps_, numPoints_] := (V0Vector = Table[v0, {k, 1, nb}];
    probden = Table[{x, ProbDensityXT[x, t, x0, sig2, nb, Nterms,
          V0Vector, xrVector, bVector, eps]} // N, {x, 0, L, L / numPoints}];
    xProb = xProbMax[probden];
    Print[xProb];
    xProb[[1]]);
```

Example for $x_0 = L/2$ and σ^2≡0.05, n_b=L=10, b =1/6 and N=100

In[75]:=
```
x0 = L / 2.; sig2 = 0.05;
nb = 10; L = N[nb]; q = 1. / 6;
{xrVector = Table[-1. / 2 + k, {k, 1, nb}], bVector = Table[q, {k, 1, nb}]};
Nterms = 100;
```

Table of {t,x_{max}} for the case where V_0=v0=0 and V_e(x)=ϵx with ϵ=eps=10

In[79]:=
```
v0 = 0.; eps = 10.; xmaxt = Table[{t, xMaxt[t, v0, eps, 200]}, {t, 0, 0.26, 0.02}]
```

```
{5., 2.52313}
{5., 1.96985}
{5., 1.33534}
{4.95, 0.969873}
{4.95, 0.752325}
{4.9, 0.61195}
{4.85, 0.514588}
{4.8, 0.443539}
{4.75, 0.389507}
{4.7, 0.347028}
{4.6, 0.312956}
{4.5, 0.284858}
{4.45, 0.261442}
{4.4, 0.241396}
```

Out[79]=
```
{{0., 5.}, {0.02, 5.}, {0.04, 5.}, {0.06, 4.95},
 {0.08, 4.95}, {0.1, 4.9}, {0.12, 4.85}, {0.14, 4.8}, {0.16, 4.75},
 {0.18, 4.7}, {0.2, 4.6}, {0.22, 4.5}, {0.24, 4.45}, {0.26, 4.4}}
```

Comparison of $x_{max}(t)$ of the wave packet with the Newton's second law prediction, $x_{max}(t)=L/2-\epsilon t^2$

In[80]:=
```
xmaxtPlot = ListPlot[xmaxt];
xmatTeo = Plot[L / 2 - eps * t^2, {t, 0, 0.35}]; Show[xmaxtPlot, xmatTeo]
```

Out[80]=