Numerical matrix method for quantum periodic potentials

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Mathematica version...

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)
```

Surface states

Functions that for a KP potential with lattice parameter a=1 and n_b barriers:

(I) evaluate the Hamiltonian matrix H_{nm} [Eq. (17)]

(II) solve Eq. (10) to find the eigenenergies and eigenfunctions.

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
```

The function *HamiltonianMatrix* provides the $N \times N$ Hamiltonian matrix for the KP potential given by xrV, bV and V0V, where N=Nterms

In[9]:=
```
HamiltonianMatrix[Nterms_, L_, V0V_, xrV_, bV_] :=
 Table[If[n == m, HHnn[n, L, V0V, xrV, bV], HHnm[n, m, L, V0V, xrV, bV]],
  {n, 1, Nterms}, {m, 1, Nterms}]
```

The function *soluKP* provides the solution of Eq. (13).
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[10]:=
```
soluKP[Nterms_, L_, V0V_, xrV_, bV_] := soluKP[Nterms, L, V0V, xrV, bV] =
  Eigensystem[N[HamiltonianMatrix[Nterms, L, V0V, xrV, bV]]] // Chop //
    Transpose // Sort // Transpose
```

In[11]:=
```
EnV[Nterms_, L_, V0V_, xrV_, bV_] :=
 EnV[Nterms, L, V0V, xrV, bV] = soluKP[Nterms, L, V0V, xrV, bV][[1]]
```

In[12]:=
```
cnMatrix[Nterms_, L_, V0V_, xrV_, bV_] :=
 cnMatrix[Nterms, L, V0V, xrV, bV] = soluKP[Nterms, L, V0V, xrV, bV][[2]]
```

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

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

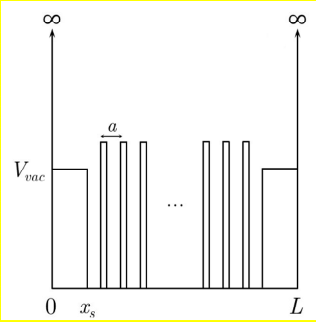
When Nast=N^* is equal to Nterm=N, this expression is just Eq. (14).
The function ProbDensity is just $|\psi_n(\mathrm{x})|^2$

In[13]:=
```
psi[n_, x_, Nast_, Nterms_, L_, V0V_, xrV_, bV_] := Sqrt[2 / L] *
  Sum[cnMatrix[Nterms, L, V0V, xrV, bV][[n, m]] * Sin[m * Pi * x / L], {m, 1, Nast}]
```

In[14]:=
```
ProbDensity[n_, x_, Nast_, Nterms_, L_, V0V_, xrV_, bV_] :=
 Abs[psi[n, x, Nast, Nterms, L, V0V, xrV, bV]]^2
```

Definition of the dimerized KP system and plot of the potential for the case with b=1/6 considered in Fig. 8

We generate the list of positions, widths and heights of the barriers that define the KP potential of Fig. 7:



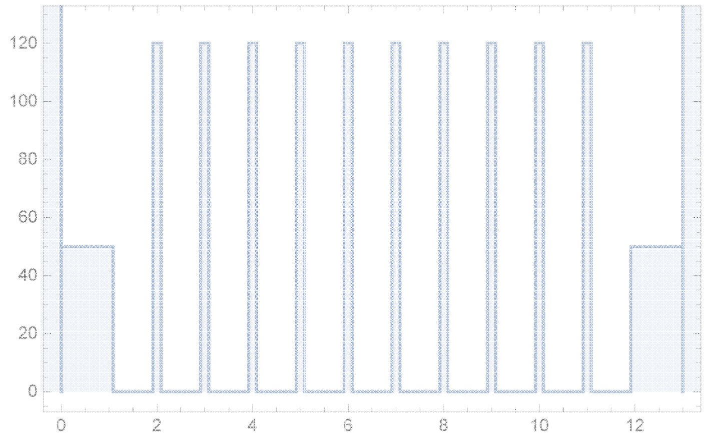
In this *example* the internal nb=10 barriers of width b=q=1/6 and heigth V_0=v0=2P/q=120 [P=10] are placed at x=2,3,...11.
Besides we stick two barriers of height V_{vac} =Vvac=50 and width 1+q/2 to the walls of the infinite square well of size L=nb+3=13

In[15]:=
```
Vvac = 50;
nb = 10;  L = N[nb] + 3; PP = 10;
 q = 1./6; v0 = 2. * PP / q;
{xrVector = Table[k, {k, 1, Round[L - 1]}], bVector = Table[q, {k, 1, Round[L - 1]}],
  V0Vector = Table[v0, {k, 1, Round[L - 1]}]};
xrVector[[1]] = (1 + q/2.) / 2.; bVector[[1]] = 1 + q/2.;
xrVector[[Length[xrVector]]] = L - (1 + q/2) / 2;
bVector[[Length[xrVector]]] = 1 + q/2.;
V0Vector[[1]] = Vvac;  V0Vector[[Length[xrVector]]] = Vvac;
```

The next instruction generates a plot of the potential defined above

```
leftWall = Plot[If[x < 0, 1.2 * v0, 0],
   {x, -1, 0.01}, Filling → Bottom, PlotPoints → 100, Frame → True];
rightWall = Plot[If[x > L, 1.2 * v0, 0], {x, L - 0.01, L + 1},
  Filling → Bottom, PlotPoints → 100, Frame → True];
KPpotential = Plot[Piecewise[Table[{V0Vector[[k]],
      xrVector[[k]] - bVector[[k]] / 2 <= x <= xrVector[[k]] + bVector[[k]] / 2},
     {k, 1, L - 1}]], {x, 0, L}, Filling → Bottom, PlotPoints → 4000, Frame → True];
Show[leftWall, rightWall, KPpotential, PlotRange → {{-0.1, L + 0.1}, {0, 1.05 v0}}]
```

Out[23]=



Evaluation of the functions $R(x) = |\Psi_1(x)|^2 / |\Psi_1(0)|^2$ for the cases considered in Fig. 8: n_b=10, V_{vac} =50, P=10, N=400 and V_0=2P/b, with b=1/6, 1/12 and 1/96

Case with b=1/6

We define the system

In[24]:=

```
q = 1. / 6;
PP = 10; v0 = 2. * PP / q;
Vvac = 50;
nb = 10;  L = N[nb] + 3;
{xrVector = Table[k, {k, 1, Round[L - 1]}], bVector = Table[q, {k, 1, Round[L - 1]}],
  V0Vector = Table[v0, {k, 1, Round[L - 1]}]};
xrVector[[1]] = (1 + q / 2.) / 2.; bVector[[1]] = 1 + q / 2.;
xrVector[[Length[xrVector]]] = L - (1 + q / 2) / 2;
bVector[[Length[xrVector]]] = 1 + q / 2.;
V0Vector[[1]] = Vvac;  V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[32]:= **Nterms = 400; Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]**

Out[32]=
```
{8.22397, 8.22959, 8.40981, 8.59389, 8.84349, 9.14209, 9.47005, 9.80279, 10.1111,
 10.3632, 10.5293, 31.9122, 31.9178, 33.0978, 33.826, 34.8436, 36.0656, 37.4144,
 38.8026, 40.1226, 41.2404, 42.0031, 56.8054, 56.8054, 68.7958, 68.7989,
 72.8295, 74.374, 76.554, 79.1377, 81.937, 84.7461, 87.2903, 89.3355, 91.055,
 92.7735, 94.2494, 116.149, 116.154, 126.676, 129.352, 132.912, 136.837,
 140.801, 144.692, 148.662, 152.935, 157.525, 162.155, 166.152, 181.916,
 182.012, 195.452, 200.115, 205.626, 211.372, 217.151, 222.993, 229.051,
 235.454, 242.216, 249.24, 256.261, 267.687, 268.943, 282.015, 289.339,
 296.98, 304.677, 312.402, 320.214, 328.201, 336.43, 344.927, 353.684, 362.71,
 372.752, 378.327, 389.664, 399.093, 408.515, 417.978, 427.512, 437.142,
 446.885, 456.753, 466.744, 476.852, 487.055, 497.25, 508.72, 518.9, 529.62,
 540.534, 551.605, 562.807, 574.112, 585.489, 596.907, 608.343, 619.777,
 631.167, 642.203, 658.447, 668.514, 680.414, 692.774, 705.39, 718.178,
 731.073, 744.019, 756.969, 769.893, 782.773, 795.57, 807.949, 826.918,
 837.801, 851.097, 864.954, 879.1, 893.428, 907.864, 922.35, 936.843, 951.318,
 965.77, 980.172, 994.252, 1014.1, 1026.63, 1041.54, 1056.94, 1072.6, 1088.44,
 1104.38, 1120.39, 1136.43, 1152.5, 1168.6, 1184.72, 1200.69, 1220.27, 1235.16,
 1251.78, 1268.73, 1285.88, 1303.19, 1320.61, 1338.12, 1355.72, 1373.39,
 1391.15, 1408.99, 1426.88, 1445.84, 1463.53, 1481.84, 1500.33, 1518.95, 1537.7,
 1556.58, 1575.59, 1594.73, 1613.99, 1633.38, 1652.91, 1672.62, 1691.24,
 1711.79, 1731.73, 1751.72, 1771.81, 1792.01, 1812.35, 1832.85, 1853.5,
 1874.33, 1895.31, 1916.45, 1937.86, 1956.78, 1979.87, 2001.36, 2022.86,
 2044.42, 2066.1, 2087.91, 2109.9, 2132.07, 2154.42, 2176.95, 2199.65, 2222.62,
 2242.61, 2267.65, 2290.67, 2313.68, 2336.76, 2359.93, 2383.25, 2406.74,
 2430.42, 2454.28, 2478.3, 2502.49, 2526.93, 2548.75, 2575.09, 2599.63, 2624.17,
 2648.78, 2673.5, 2698.35, 2723.35, 2748.53, 2773.86, 2799.36, 2825., 2850.84,
 2875.07, 2902.2, 2928.24, 2954.33, 2980.5, 3006.78, 3033.18, 3059.71, 3086.38,
 3113.19, 3140.13, 3167.2, 3194.41, 3221.35, 3249.03, 3276.56, 3304.19,
 3331.93, 3359.78, 3387.74, 3415.8, 3443.97, 3472.25, 3500.64, 3529.14,
 3557.72, 3587.36, 3615.62, 3644.63, 3673.8, 3703.1, 3732.52, 3762.03, 3791.63,
 3821.31, 3851.08, 3880.93, 3910.88, 3940.88, 3972.87, 4001.99, 4032.48,
 4063.18, 4094.03, 4124.99, 4156.05, 4187.18, 4218.39, 4249.66, 4281.01,
 4312.45, 4343.94, 4377.76, 4408.13, 4440.12, 4472.34, 4504.72, 4537.21,
 4569.8, 4602.46, 4635.2, 4668., 4700.89, 4733.86, 4766.89, 4801.98, 4834.04,
 4867.56, 4901.29, 4935.17, 4969.17, 5003.27, 5037.46, 5071.73, 5106.08,
 5140.53, 5175.09, 5209.71, 5245.63, 5279.73, 5314.79, 5350.02, 5385.39,
 5420.88, 5456.48, 5492.19, 5527.99, 5563.91, 5599.93, 5636.06, 5672.29,
 5708.85, 5745.18, 5781.78, 5818.51, 5855.36, 5892.33, 5929.42, 5966.64,
 6003.98, 6041.45, 6079.04, 6116.78, 6154.63, 6191.84, 6230.43, 6268.56,
 6306.78, 6345.11, 6383.56, 6422.15, 6460.87, 6499.74, 6538.75, 6577.9,
 6617.17, 6656.59, 6694.74, 6735.36, 6775.02, 6814.75, 6854.57, 6894.52,
 6934.6, 6974.83, 7015.22, 7055.76, 7096.44, 7137.32, 7178.28, 7217.73,
 7260.09, 7301.28, 7342.51, 7383.85, 7425.3, 7466.9, 7508.64, 7550.53, 7592.58,
 7634.76, 7677.07, 7719.53, 7760.7, 7804.41, 7847.12, 7889.89, 7932.75,
 7975.74, 8018.85, 8062.11, 8105.51, 8149.06, 8192.73, 8236.74, 8280.67,
```

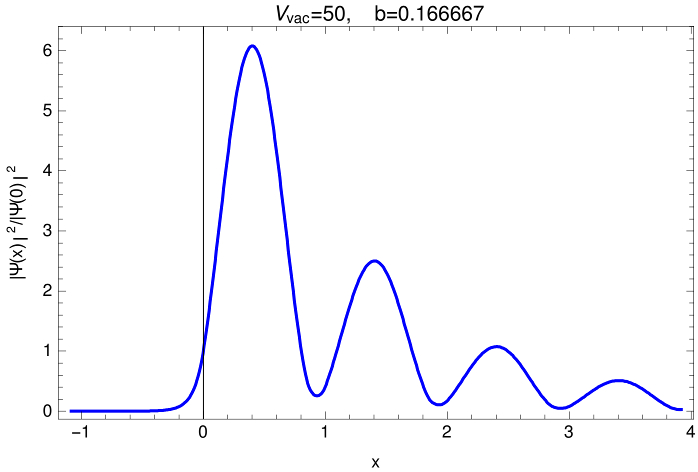
```
8323.88, 8368.67, 8412.9, 8457.21, 8501.63, 8546.16, 8590.81, 8635.58,
8680.48, 8725.51, 8770.66, 8815.93, 8861.32, 8906.75, 8952.44, 8998.17,
9044.04, 9090.01, 9136.12, 9182.31, 9228.67, 9275.08, 9321.74, 9368.37}
```

RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

```
In[33]:= xsLeft = 1 + q / 2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
      Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q (in this case Vvac=50 and q=1/6)

```
In[34]:= RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|^2/|Ψ(0)|^2"}, PlotRange → All,
  PlotLabel → StringJoin[{" Vvac=", ToString[Vvac] , ",     b=", ToString[q]}],
  PlotStyle → Blue, Joined → True]
```

Out[34]=


Case with b=1/12

We define the system

```
In[35]:= q = 1. / 12;
PP = 10; v0 = 2. * PP / q;
Vvac = 50;
nb = 10;  L = N[nb] + 3;
{xrVector = Table[k, {k, 1, Round[L - 1]}], bVector = Table[q, {k, 1, Round[L - 1]}],
  V0Vector = Table[v0, {k, 1, Round[L - 1]}]};
xrVector[[1]] = (1 + q / 2.) / 2.; bVector[[1]] = 1 + q / 2.;
xrVector[[Length[xrVector]]] = L - (1 + q / 2) / 2;
bVector[[Length[xrVector]]] = 1 + q / 2.;
V0Vector[[1]] = Vvac;  V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[43]:=
```
Nterms = 400; Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]
```

Out[43]=
```
{7.37018, 7.37226, 7.6405, 7.83377, 8.10474, 8.43315, 8.79748, 9.17083, 9.52038,
 9.80912, 10.0008, 28.9946, 28.9966, 30.6839, 31.4203, 32.4739, 33.7475,
 35.1555, 36.6071, 37.9914, 39.1689, 39.9766, 55.9362, 55.9362, 65.9341,
 65.9383, 69.5575, 71.1196, 73.3149, 75.9188, 78.7613, 81.6808, 84.4849,
 86.9075, 88.6339, 89.639, 90.2856, 114.067, 114.07, 124.802, 127.322, 130.748,
 134.578, 138.406, 141.957, 145.327, 148.908, 152.817, 156.676, 159.741,
 180.83, 180.844, 197.224, 200.99, 205.793, 210.881, 215.884, 220.85, 226.113,
 231.866, 237.964, 243.997, 249.121, 267.347, 267.434, 287.559, 292.92, 299.333,
 305.945, 312.52, 319.237, 326.395, 334.092, 342.18, 350.342, 357.851, 373.902,
 374.3, 396.474, 403.742, 411.934, 420.238, 428.543, 437.063, 446.045, 455.558,
 465.497, 475.648, 485.563, 500.423, 501.707, 524.569, 533.935, 543.958,
 554.018, 564.102, 574.417, 585.161, 596.397, 608.057, 620.007, 632.043,
 646.715, 649.761, 672.311, 683.8, 695.636, 707.458, 719.32, 731.401, 743.856,
 756.738, 770.012, 783.594, 797.402, 812.606, 818.294, 840.022, 853.515,
 867.101, 880.66, 894.275, 908.087, 922.206, 936.679, 951.487, 966.578,
 981.917, 998.03, 1007.01, 1027.84, 1043.15, 1058.42, 1073.68, 1089.02,
 1104.52, 1120.27, 1136.29, 1152.58, 1169.11, 1185.85, 1203.03, 1215.65,
 1235.78, 1252.73, 1269.63, 1286.55, 1303.57, 1320.73, 1338.08, 1355.62,
 1373.36, 1391.29, 1409.37, 1427.7, 1444.03, 1463.76, 1482.22, 1500.71,
 1519.27, 1537.94, 1556.73, 1575.65, 1594.7, 1613.88, 1633.19, 1652.62,
 1672.15, 1692.06, 1711.69, 1731.61, 1751.66, 1771.83, 1792.12, 1812.51,
 1832.98, 1853.53, 1874.16, 1894.87, 1915.65, 1936.45, 1959.63, 1979.5,
 2000.85, 2022.45, 2044.21, 2066.09, 2088.05, 2110.07, 2132.12, 2154.21,
 2176.34, 2198.52, 2220.65, 2246.72, 2267.13, 2289.92, 2313.06, 2336.39,
 2359.84, 2383.37, 2406.92, 2430.48, 2454.03, 2477.61, 2501.23, 2524.75,
 2553.27, 2574.53, 2598.79, 2623.46, 2648.34, 2673.35, 2698.42, 2723.51,
 2748.57, 2773.63, 2798.68, 2823.78, 2848.78, 2879.31, 2901.69, 2927.46,
 2953.66, 2980.08, 3006.62, 3033.23, 3059.83, 3086.42, 3112.99, 3139.56,
 3166.16, 3192.68, 3224.81, 3248.59, 3275.89, 3303.61, 3331.55, 3359.62,
 3387.75, 3415.88, 3443.99, 3472.09, 3500.2, 3528.37, 3556.46, 3589.82,
 3615.26, 3644.11, 3673.35, 3702.8, 3732.38, 3762.01, 3791.66, 3821.31,
 3850.95, 3880.62, 3910.35, 3940.05, 3974.35, 4001.67, 4032.07, 4062.83,
 4093.77, 4124.85, 4155.99, 4187.16, 4218.34, 4249.54, 4280.79, 4312.13,
 4343.45, 4378.49, 4407.87, 4439.83, 4472.09, 4504.53, 4537.08, 4569.72,
 4602.4, 4635.12, 4667.89, 4700.72, 4733.63, 4766.59, 4802.23, 4833.81,
 4867.32, 4901.08, 4934.99, 4969.03, 5003.15, 5037.35, 5071.61, 5105.95,
 5140.36, 5174.92, 5209.51, 5245.69, 5279.56, 5314.62, 5349.87, 5385.25,
 5420.76, 5456.37, 5492.08, 5527.88, 5563.78, 5599.78, 5635.89, 5672.11,
 5708.84, 5745.02, 5781.62, 5818.35, 5855.21, 5892.19, 5929.28, 5966.5,
 6003.84, 6041.31, 6078.89, 6116.66, 6154.49, 6191.83, 6230.32, 6268.44,
 6306.66, 6344.99, 6383.43, 6422.02, 6460.75, 6499.62, 6538.64, 6577.79,
 6617.07, 6656.49, 6694.59, 6735.28, 6774.92, 6814.63, 6854.43, 6894.36,
 6934.43, 6974.67, 7015.07, 7055.65, 7096.36, 7137.32, 7178.31, 7217.28,
```

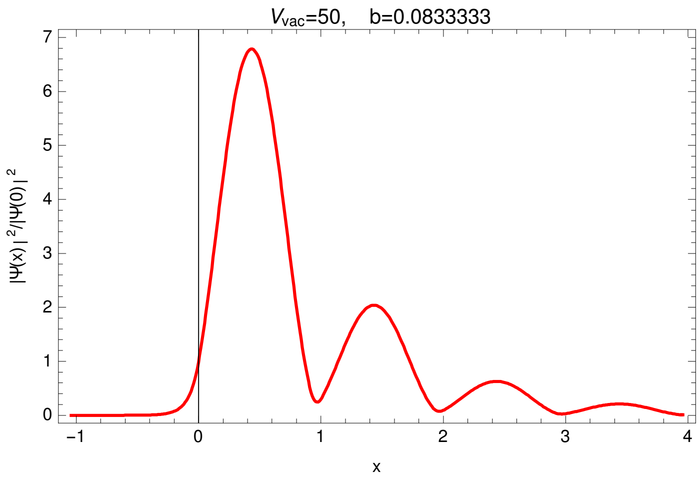
```
7260.1, 7301.26, 7342.45, 7383.73, 7425.15, 7466.72, 7508.46, 7550.39, 7592.5,
7634.76, 7677.16, 7719.71, 7759.77, 7804.51, 7847.18, 7889.88, 7932.66,
7975.56, 8018.63, 8061.89, 8105.34, 8148.99, 8192.79, 8236.97, 8281.06,
8322.33, 8368.92, 8413.11, 8457.29, 8501.58, 8545.99, 8590.57, 8635.34,
8680.32, 8725.48, 8770.81, 8816.27, 8861.88, 8904.61, 8952.77, 8998.47,
9044.21, 9090.01, 9135.98, 9182.07, 9228.42, 9274.91, 9321.73, 9368.56}
```

RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

In[44]:=
```
xsLeft = 1 + q / 2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
     Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q (in this case Vvac=50 and q=1/12)

In[45]:=
```
RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|²/|Ψ(0)|²"}, PlotRange → All,
  PlotLabel → StringJoin[{" Vvac=", ToString[Vvac] , ",     b=", ToString[q]}],
  PlotStyle → Red, Joined → True]
```

Out[45]=


Case with b=1/96

We define the system

In[46]:=
```
q = 1. / 96;
PP = 10; v0 = 2. * PP / q;
Vvac = 50;
nb = 10;  L = N[nb] + 3;
{xrVector = Table[k, {k, 1, Round[L - 1]}], bVector = Table[q, {k, 1, Round[L - 1]}],
  V0Vector = Table[v0, {k, 1, Round[L - 1]}]};
xrVector[[1]] = (1 + q / 2.) / 2.; bVector[[1]] = 1 + q / 2.;
xrVector[[Length[xrVector]]] = L - (1 + q / 2) / 2;
bVector[[Length[xrVector]]] = 1 + q / 2.;
V0Vector[[1]] = Vvac;  V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[54]:=
```
Nterms = 400; Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]
```

Out[54]=
```
{6.7741, 6.77502, 7.14114, 7.34667, 7.64246, 8.00563, 8.41293, 8.83503, 9.23517,
 9.56957, 9.79401, 26.859, 26.8622, 29.0242, 29.8038, 30.9273, 32.3008, 33.8246,
 35.406, 36.9296, 38.2444, 39.1602, 54.5901, 54.5902, 64.0419, 64.0535,
 66.7784, 68.4643, 70.7873, 73.5259, 76.5147, 79.6029, 82.6201, 85.3391,
 87.4715, 88.8032, 89.0582, 111.581, 111.59, 121.544, 124.235, 127.838,
 131.907, 136.032, 139.85, 143.215, 146.498, 150.099, 153.785, 156.769,
 178.736, 178.752, 194.334, 198.203, 203.142, 208.379, 213.443, 218.242,
 223.15, 228.541, 234.34, 240.064, 244.808, 265.538, 265.595, 285.959, 291.122,
 297.382, 303.86, 310.146, 316.412, 323.1, 330.398, 338.101, 345.744, 352.365,
 372.19, 372.343, 396.623, 403.213, 410.94, 418.766, 426.455, 434.306, 442.731,
 451.814, 461.326, 470.836, 479.425, 498.739, 499.093, 526.804, 534.871,
 544.017, 553.264, 562.435, 571.895, 582.01, 592.813, 604.071, 615.397,
 625.954, 645.133, 645.824, 676.39, 686.013, 696.707, 707.42, 718.113, 729.179,
 740.951, 753.429, 766.394, 779.486, 791.998, 811.375, 812.555, 845.734,
 856.914, 869.07, 881.275, 893.507, 906.173, 919.575, 933.702, 948.335,
 963.152, 977.533, 997.392, 999.226, 1034.61, 1047.39, 1061.13, 1074.84,
 1088.62, 1102.88, 1117.9, 1133.65, 1149.93, 1166.43, 1182.65, 1203.22, 1205.83,
 1243.33, 1257.7, 1272.91, 1288.14, 1303.47, 1319.31, 1335.93, 1353.28,
 1371.19, 1389.35, 1407.32, 1428.77, 1432.32, 1471.61, 1487.61, 1504.41,
 1521.17, 1538.05, 1555.47, 1573.67, 1592.62, 1612.13, 1631.93, 1651.64,
 1674.12, 1678.67, 1719.79, 1737.37, 1755.65, 1773.94, 1792.37, 1811.36,
 1831.14, 1851.68, 1872.78, 1894.19, 1915.55, 1939.17, 1944.84, 1987.54,
 2006.74, 2026.62, 2046.44, 2066.43, 2086.99, 2108.33, 2130.44, 2153.13,
 2176.14, 2199.18, 2224.01, 2230.84, 2275.2, 2295.99, 2317.33, 2338.69,
 2360.23, 2382.35, 2405.26, 2428.94, 2453.2, 2477.8, 2502.43, 2528.53, 2536.63,
 2582.44, 2604.84, 2627.78, 2650.68, 2673.77, 2697.44, 2721.91, 2747.15,
 2772.98, 2799.16, 2825.43, 2852.85, 2862.21, 2909.59, 2933.56, 2957.98,
 2982.41, 3007.05, 3032.28, 3058.31, 3085.1, 3112.49, 3140.24, 3168.05, 3196.85,
 3207.56, 3256.31, 3281.89, 3307.91, 3333.88, 3360.07, 3386.85, 3414.43,
 3442.77, 3471.72, 3501.03, 3530.47, 3560.65, 3572.7, 3622.97, 3650.12, 3677.6,
 3705.11, 3732.84, 3761.17, 3790.3, 3820.19, 3850.69, 3881.55, 3912.5, 3944.1,
 3957.59, 4009.18, 4037.93, 4067.02, 4096.06, 4125.34, 4155.22, 4185.89,
```

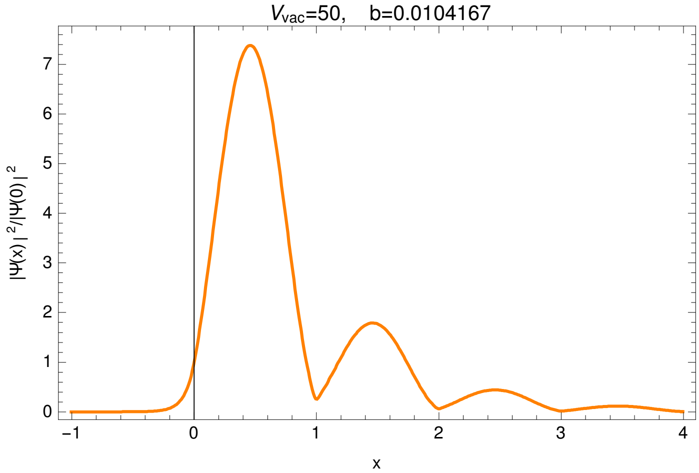
```
4217.33, 4249.38, 4281.79, 4314.36, 4347.38, 4362.25, 4415.36, 4445.65,
4476.2, 4506.78, 4537.6, 4569.03, 4601.24, 4634.22, 4667.81, 4701.77, 4735.83,
4770.3, 4786.66, 4841.05, 4872.94, 4905.11, 4937.22, 4969.59, 5002.56,
5036.32, 5070.84, 5105.96, 5141.46, 5177.15, 5213.07, 5230.83, 5286.75,
5320.18, 5353.78, 5387.43, 5421.34, 5455.85, 5491.15, 5527.21, 5563.87,
5600.91, 5638.06, 5675.46, 5694.75, 5751.93, 5786.95, 5822.18, 5857.37,
5892.82, 5928.87, 5965.71, 6003.3, 6041.5, 6080.08, 6118.87, 6157.73, 6178.44,
6237.18, 6273.73, 6310.36, 6347.08, 6384.07, 6421.66, 6460.03, 6499.17,
6538.9, 6579.01, 6619.23, 6659.58, 6681.86, 6741.83, 6779.97, 6818.27,
6856.53, 6895.06, 6934.18, 6974.09, 7014.75, 7056.02, 7097.67, 7139.58,
7181.4, 7205.05, 7266.72, 7306.36, 7345.98, 7385.77, 7425.83, 7466.5, 7507.94,
7550.14, 7592.94, 7636.12, 7679.4, 7722.72, 7747.97, 7810.84, 7852.07,
7893.42, 7934.74, 7976.34, 8018.54, 8061.52, 8105.25, 8149.6, 8194.31,
8239.45, 8284.25, 8310.66, 8375.7, 8418.4, 8460.79, 8503.62, 8546.74, 8590.48,
8635., 8680.28, 8726.16, 8772.42, 8818.77, 8865.07, 8893.1, 8959.27, 9003.56,
9047.98, 9092.39, 9137.11, 9182.45, 9228.62, 9275.53, 9323.28, 9371.34}
```

RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

In[55]:=
```
xsLeft = 1 + q / 2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
      Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q (in this case Vvac=50 and q=1/96)

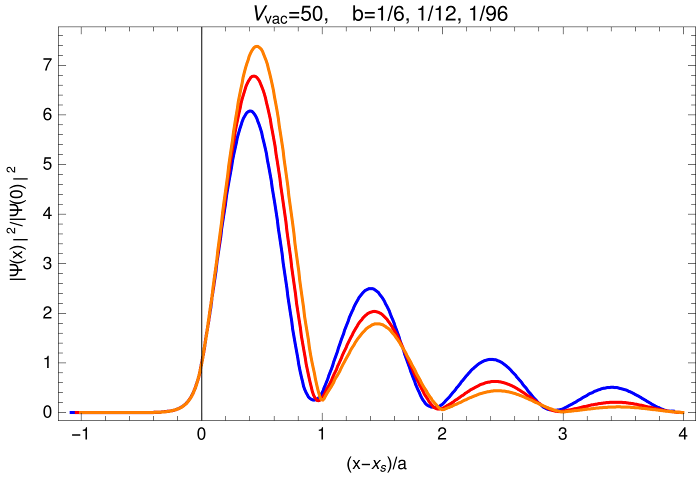
In[56]:=
```
RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|²/|Ψ(0)|²"}, PlotRange → All,
  PlotLabel → StringJoin[{" Vvac=", ToString[Vvac] , ",     b=", ToString[q]}],
  PlotStyle → Orange, Joined → True]
```

Out[56]=


We combine and compare the function $R(x) = |\Psi_1(x)|^2 / |\Psi_1(0)|^2$ for these three cases

In[57]:=
```
Show[{RxPlot[50, 1. / 6], RxPlot[50, 1. / 12], RxPlot[50, 1. / 96]},
 PlotRange → All, FrameLabel -> {"(x-xs)/a", "|Ψ(x)|^2/|Ψ(0)|^2"}, PlotLabel →
  StringJoin[{" Vvac=", ToString[Vvac] , ",     b=", "1/6, 1/12, 1/96"}]]
```

Out[57]=



Relative probability $R(x) = |\Psi_1(x)|^2 / |\Psi_1(0)|^2$ for several values of V_{vac} when n_b=10, P=10, V_0=2P/b with b=1/96, and N=400

We define the system and the value of N

In[58]:=
```
Nterms = 400;
q = 1. / 96;
PP = 10; v0 = 2. * PP / q;
nb = 10;  L = N[nb] + 3;
{xrVector = Table[k, {k, 1, Round[L - 1]}], bVector = Table[q, {k, 1, Round[L - 1]}],
  V0Vector = Table[v0, {k, 1, Round[L - 1]}]};
xrVector[[1]] = (1 + q / 2.) / 2.; bVector[[1]] = 1 + q / 2.;
xrVector[[Length[xrVector]]] = L - (1 + q / 2) / 2;
bVector[[Length[xrVector]]] = 1 + q / 2.;
```

R(x) for Vvac=50

In[65]:=
```
Vvac = 50;
V0Vector[[1]] = Vvac;  V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[67]:=
```
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]
```

Out[67]=
```
{6.7741, 6.77502, 7.14114, 7.34667, 7.64246, 8.00563, 8.41293, 8.83503, 9.23517,
 9.56957, 9.79401, 26.859, 26.8622, 29.0242, 29.8038, 30.9273, 32.3008, 33.8246,
 35.406, 36.9296, 38.2444, 39.1602, 54.5901, 54.5902, 64.0419, 64.0535,
 66.7784, 68.4643, 70.7873, 73.5259, 76.5147, 79.6029, 82.6201, 85.3391,
 87.4715, 88.8032, 89.0582, 111.581, 111.59, 121.544, 124.235, 127.838,
```

131.907, 136.032, 139.85, 143.215, 146.498, 150.099, 153.785, 156.769,
178.736, 178.752, 194.334, 198.203, 203.142, 208.379, 213.443, 218.242,
223.15, 228.541, 234.34, 240.064, 244.808, 265.538, 265.595, 285.959, 291.122,
297.382, 303.86, 310.146, 316.412, 323.1, 330.398, 338.101, 345.744, 352.365,
372.19, 372.343, 396.623, 403.213, 410.94, 418.766, 426.455, 434.306, 442.731,
451.814, 461.326, 470.836, 479.425, 498.739, 499.093, 526.804, 534.871,
544.017, 553.264, 562.435, 571.895, 582.01, 592.813, 604.071, 615.397,
625.954, 645.133, 645.824, 676.39, 686.013, 696.707, 707.42, 718.113, 729.179,
740.951, 753.429, 766.394, 779.486, 791.998, 811.375, 812.555, 845.734,
856.914, 869.07, 881.275, 893.507, 906.173, 919.575, 933.702, 948.335,
963.152, 977.533, 997.392, 999.226, 1034.61, 1047.39, 1061.13, 1074.84,
1088.62, 1102.88, 1117.9, 1133.65, 1149.93, 1166.43, 1182.65, 1203.22, 1205.83,
1243.33, 1257.7, 1272.91, 1288.14, 1303.47, 1319.31, 1335.93, 1353.28,
1371.19, 1389.35, 1407.32, 1428.77, 1432.32, 1471.61, 1487.61, 1504.41,
1521.17, 1538.05, 1555.47, 1573.67, 1592.62, 1612.13, 1631.93, 1651.64,
1674.12, 1678.67, 1719.79, 1737.37, 1755.65, 1773.94, 1792.37, 1811.36,
1831.14, 1851.68, 1872.78, 1894.19, 1915.55, 1939.17, 1944.84, 1987.54,
2006.74, 2026.62, 2046.44, 2066.43, 2086.99, 2108.33, 2130.44, 2153.13,
2176.14, 2199.18, 2224.01, 2230.84, 2275.2, 2295.99, 2317.33, 2338.69,
2360.23, 2382.35, 2405.26, 2428.94, 2453.2, 2477.8, 2502.43, 2528.53, 2536.63,
2582.44, 2604.84, 2627.78, 2650.68, 2673.77, 2697.44, 2721.91, 2747.15,
2772.98, 2799.16, 2825.43, 2852.85, 2862.21, 2909.59, 2933.56, 2957.98,
2982.41, 3007.05, 3032.28, 3058.31, 3085.1, 3112.49, 3140.24, 3168.05, 3196.85,
3207.56, 3256.31, 3281.89, 3307.91, 3333.88, 3360.07, 3386.85, 3414.43,
3442.77, 3471.72, 3501.03, 3530.47, 3560.65, 3572.7, 3622.97, 3650.12, 3677.6,
3705.11, 3732.84, 3761.17, 3790.3, 3820.19, 3850.69, 3881.55, 3912.5, 3944.1,
3957.59, 4009.18, 4037.93, 4067.02, 4096.06, 4125.34, 4155.22, 4185.89,
4217.33, 4249.38, 4281.79, 4314.36, 4347.38, 4362.25, 4415.36, 4445.65,
4476.2, 4506.78, 4537.6, 4569.03, 4601.24, 4634.22, 4667.81, 4701.77, 4735.83,
4770.3, 4786.66, 4841.05, 4872.94, 4905.11, 4937.22, 4969.59, 5002.56,
5036.32, 5070.84, 5105.96, 5141.46, 5177.15, 5213.07, 5230.83, 5286.75,
5320.18, 5353.78, 5387.43, 5421.34, 5455.85, 5491.15, 5527.21, 5563.87,
5600.91, 5638.06, 5675.46, 5694.75, 5751.93, 5786.95, 5822.18, 5857.37,
5892.82, 5928.87, 5965.71, 6003.3, 6041.5, 6080.08, 6118.87, 6157.73, 6178.44,
6237.18, 6273.73, 6310.36, 6347.08, 6384.07, 6421.66, 6460.03, 6499.17,
6538.9, 6579.01, 6619.23, 6659.58, 6681.86, 6741.83, 6779.97, 6818.27,
6856.53, 6895.06, 6934.18, 6974.09, 7014.75, 7056.02, 7097.67, 7139.58,
7181.4, 7205.05, 7266.72, 7306.36, 7345.98, 7385.77, 7425.83, 7466.5, 7507.94,
7550.14, 7592.94, 7636.12, 7679.4, 7722.72, 7747.97, 7810.84, 7852.07,
7893.42, 7934.74, 7976.34, 8018.54, 8061.52, 8105.25, 8149.6, 8194.31,
8239.45, 8284.25, 8310.66, 8375.7, 8418.4, 8460.79, 8503.62, 8546.74, 8590.48,
8635., 8680.28, 8726.16, 8772.42, 8818.77, 8865.07, 8893.1, 8959.27, 9003.56,
9047.98, 9092.39, 9137.11, 9182.45, 9228.62, 9275.53, 9323.28, 9371.34}

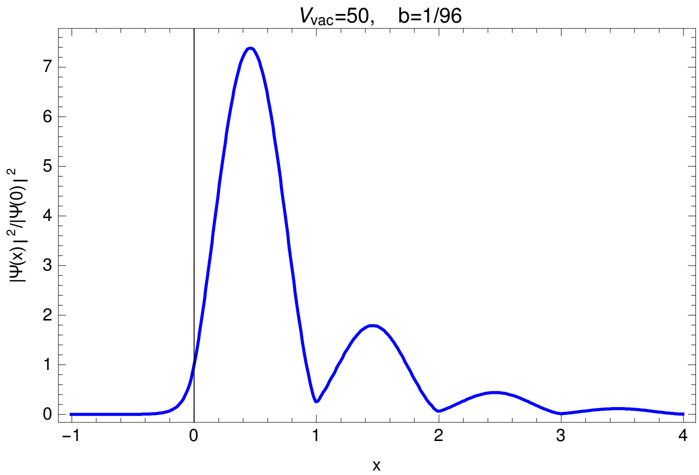
RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

In[68]:=
```
xsLeft = 1 + q/2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
      Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q (in this case Vvac=50 and q=1/6)

In[69]:=
```
RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|^2/|Ψ(0)|^2"}, PlotRange → All,
  PlotLabel → StringJoin[{" V_vac=", ToString[Vvac] , ",     b=", "1/96"}],
  PlotStyle → Blue, Joined → True]
```

Out[69]=



R(x) for Vvac=90

In[70]:=
```
Vvac = 90;
V0Vector[[1]] = Vvac;  V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[72]:=
```
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]
```

Out[72]=
```
{7.03073, 7.05529, 7.20151, 7.42232, 7.71797, 8.07402, 8.47005, 8.87814, 9.26319,
 9.58352, 9.79776, 28.3977, 28.4456, 29.1836, 30.0616, 31.2144, 32.5777,
 34.0707, 35.6059, 37.0712, 38.3216, 39.1826, 63.9642, 63.9853, 66.8904,
 68.7485, 71.2101, 74.0519, 77.1218, 80.2789, 83.3539, 86.0926, 88.0992,
 98.2257, 98.2268, 111.988, 111.997, 121.528, 124.117, 127.37, 130.498, 133.096,
 135.911, 139.665, 144.097, 148.713, 153.077, 156.54, 168.447, 168.462, 192.989,
 194.121, 196.803, 201.015, 206.313, 212.275, 218.611, 225.097, 231.507,
 237.518, 242.622, 246.095, 247.078, 281.085, 281.575, 287.516, 293.764,
 300.973, 308.706, 316.629, 324.462, 331.841, 338.361, 343.957, 349.053,
 353.47, 387.807, 388.265, 398.16, 406.088, 415.011, 424.303, 433.589, 442.524,
 450.823, 458.528, 466.109, 473.777, 480.635, 514.024, 514.601, 528.439,
 537.999, 548.495, 559.253, 569.827, 579.922, 589.485, 598.869, 608.534,
 618.439, 627.473, 659.882, 660.687, 678.197, 689.412, 701.509, 713.694,
 725.573, 736.958, 748.004, 759.169, 770.81, 782.753, 793.907, 825.551, 826.691,
```

```
847.703, 860.544, 874.132, 887.733, 900.954, 913.73, 926.35, 939.287, 952.795,
966.668, 979.887, 1010.98, 1012.58, 1036.76, 1051.25, 1066.4, 1081.42,
1096.02, 1110.25, 1124.49, 1139.16, 1154.47, 1170.19, 1185.45, 1216.26,
1218.45, 1245.65, 1261.74, 1278.34, 1294.79, 1310.81, 1326.54, 1342.39,
1358.78, 1375.83, 1393.34, 1410.56, 1441.31, 1444.21, 1474.12, 1491.83,
1509.98, 1527.86, 1545.33, 1562.58, 1580.05, 1598.11, 1616.87, 1636.13,
1655.27, 1686.2, 1689.92, 1722.44, 1741.74, 1761.33, 1780.66, 1799.59,
1818.37, 1837.46, 1857.18, 1877.61, 1898.57, 1919.55, 1950.83, 1955.51,
1990.36, 2011.26, 2032.39, 2053.18, 2073.59, 2093.92, 2114.61, 2135.96,
2158.05, 2180.69, 2203.49, 2235.3, 2241., 2278.15, 2300.61, 2323.18, 2345.43,
2367.34, 2389.21, 2411.5, 2434.48, 2458.19, 2482.49, 2507.02, 2539.48,
2546.33, 2585.54, 2609.58, 2633.69, 2657.42, 2680.82, 2704.25, 2728.13,
2752.72, 2778.05, 2803.97, 2830.25, 2863.5, 2871.53, 2912.81, 2938.4, 2963.95,
2989.15, 3014.06, 3039.04, 3064.5, 3090.69, 3117.63, 3145.16, 3173.08,
3207.21, 3216.54, 3259.67, 3286.82, 3313.92, 3340.62, 3367.04, 3393.57,
3420.61, 3448.39, 3476.92, 3506.06, 3535.66, 3570.77, 3581.38, 3626.43,
3655.13, 3683.65, 3711.83, 3739.77, 3767.85, 3796.47, 3825.83, 3855.94,
3886.67, 3917.85, 3953.99, 3966.01, 4012.76, 4043.01, 4073.1, 4102.78, 4132.24,
4161.87, 4192.06, 4222.99, 4254.68, 4286.98, 4319.82, 4357.08, 4370.45,
4419.03, 4450.8, 4482.31, 4513.48, 4544.46, 4575.64, 4607.39, 4639.9, 4673.16,
4707.03, 4741.4, 4779.8, 4794.66, 4844.83, 4878.15, 4911.24, 4943.91, 4976.42,
5009.15, 5042.47, 5076.54, 5111.36, 5146.79, 5182.81, 5222.41, 5238.67,
5290.6, 5325.45, 5359.93, 5394.11, 5428.14, 5462.42, 5497.29, 5532.93, 5569.3,
5606.3, 5643.8, 5684.62, 5702.44, 5755.88, 5792.27, 5828.35, 5864.04, 5899.6,
5935.42, 5971.85, 6009.04, 6046.98, 6085.52, 6124.67, 6166.77, 6186., 6241.2,
6279.09, 6316.55, 6353.74, 6390.83, 6428.19, 6466.18, 6504.92, 6544.4,
6584.49, 6625.09, 6668.47, 6689.3, 6745.94, 6785.38, 6824.47, 6863.17,
6901.79, 6940.7, 6980.23, 7020.53, 7061.56, 7103.19, 7145.48, 7190.2, 7212.39,
7270.87, 7311.81, 7352.19, 7392.4, 7432.54, 7473., 7514.08, 7555.93, 7598.5,
7641.68, 7685.36, 7731.39, 7755.22, 7815.08, 7857.56, 7899.65, 7941.38,
7983.05, 8025.04, 8067.67, 8111.06, 8155.18, 8199.9, 8245.44, 8292.88,
8317.85, 8379.96, 8423.93, 8467.04, 8510.26, 8553.43, 8596.97, 8641.16,
8686.12, 8731.81, 8778.08, 8824.84, 8873.64, 8900.26, 8963.62, 9009.12,
9054.29, 9099.09, 9144.02, 9189.21, 9235.4, 9282.05, 9330.78, 9378.97}
```

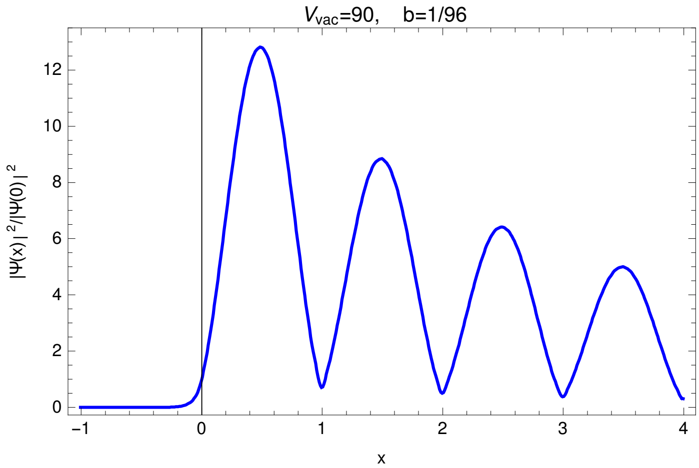
RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

In[73]:=
```
xsLeft = 1 + q / 2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
      Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q (in this case Vvac=50 and q=1/6)

In[74]:=
```
RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|²/|Ψ(0)|²"}, PlotRange → All,
  PlotLabel → StringJoin[{" Vvac=", ToString[Vvac] , ",     b=", "1/96"}],
  PlotStyle → Blue, Joined → True]
```

Out[74]=



R(x) for Vvac=100

In[75]:=
```
Vvac = 100;
V0Vector[[1]] = Vvac; V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[77]:=
```
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]
```

Out[77]=
```
{7.04969, 7.08482, 7.222, 7.44136, 7.73516, 8.08888, 8.48212, 8.8871, 9.26893,
 9.58635, 9.79851, 28.5374, 28.6158, 29.249, 30.1309, 31.2799, 32.6356, 34.1193,
 35.6436, 37.0967, 38.335, 39.1864, 64.6434, 64.6885, 66.9787, 68.889, 71.3637,
 74.2047, 77.2668, 80.4097, 83.4615, 86.1637, 88.1241, 106.36, 106.362,
 116.306, 116.334, 121.722, 124.647, 128.412, 132.573, 136.621, 139.886,
 142.43, 145.452, 149.37, 153.418, 156.66, 174.041, 174.052, 193.866, 196.417,
 199.434, 203.023, 207.662, 213.256, 219.435, 225.898, 232.393, 238.609,
 243.995, 250.552, 250.778, 283.456, 284.689, 288.856, 294.853, 301.929, 309.64,
 317.661, 325.748, 333.608, 340.803, 346.73, 351.099, 354.156, 390.812, 391.67,
 399.031, 407.012, 415.964, 425.367, 434.893, 444.228, 453.004, 460.917,
 468.103, 474.955, 481.02, 517.273, 518.131, 529.159, 538.888, 549.502,
 560.451, 571.334, 581.819, 591.656, 600.932, 610.106, 619.392, 627.836,
 663.19, 664.226, 678.884, 690.319, 702.579, 715.001, 727.203, 738.905,
 750.061, 761., 772.196, 783.653, 794.306, 828.848, 830.18, 848.381, 861.474,
 875.264, 889.125, 902.653, 915.668, 928.296, 940.976, 954.096, 967.574,
 980.351, 1014.21, 1015.97, 1037.46, 1052.22, 1067.58, 1082.87, 1097.76,
 1112.16, 1126.35, 1140.76, 1155.74, 1171.13, 1185.99, 1219.43, 1221.72,
 1246.36, 1262.74, 1279.58, 1296.29, 1312.56, 1328.42, 1344.18, 1360.32,
 1377.08, 1394.31, 1411.18, 1444.38, 1447.35, 1474.86, 1492.86, 1511.26,
 1529.4, 1547.09, 1564.42, 1581.79, 1599.62, 1618.13, 1637.14, 1655.99, 1689.19,
 1692.93, 1723.21, 1742.8, 1762.64, 1782.22, 1801.35, 1820.19, 1839.16,
 1858.67, 1878.87, 1899.63, 1920.36, 1953.73, 1958.39, 1991.16, 2012.35,
```

```
2033.73, 2054.76, 2075.34, 2095.71, 2116.28, 2137.44, 2159.32, 2181.78,
2204.38, 2238.12, 2243.76, 2278.97, 2301.74, 2324.55, 2347.03, 2369.08,
2390.98, 2413.15, 2435.94, 2459.47, 2483.61, 2507.98, 2542.22, 2548.97,
2586.39, 2610.73, 2635.09, 2659.03, 2682.57, 2706., 2729.76, 2754.18, 2779.34,
2805.13, 2831.28, 2866.18, 2874.07, 2913.68, 2939.58, 2965.36, 2990.77,
3015.8, 3040.77, 3066.12, 3092.15, 3118.93, 3146.35, 3174.17, 3209.82, 3218.98,
3260.57, 3288.02, 3315.35, 3342.24, 3368.77, 3395.29, 3422.22, 3449.84,
3478.23, 3507.27, 3536.81, 3573.32, 3583.74, 3627.35, 3656.34, 3685.09,
3713.46, 3741.49, 3769.56, 3798.07, 3827.28, 3857.26, 3887.9, 3919.05,
3956.48, 3968.29, 4013.71, 4044.25, 4074.56, 4104.41, 4133.95, 4163.57,
4193.65, 4224.45, 4256.02, 4288.24, 4321.06, 4359.52, 4372.67, 4419.99,
4452.06, 4483.77, 4515.11, 4546.17, 4577.33, 4608.98, 4641.36, 4674.5, 4708.31,
4742.68, 4782.19, 4796.82, 4845.81, 4879.43, 4912.72, 4945.55, 4978.12,
5010.83, 5044.05, 5078., 5112.71, 5148.09, 5184.11, 5224.76, 5240.78, 5291.61,
5326.73, 5361.42, 5395.74, 5429.84, 5464.09, 5498.87, 5534.39, 5570.67,
5607.61, 5645.14, 5686.93, 5704.49, 5756.9, 5793.57, 5829.85, 5865.67, 5901.29,
5937.09, 5973.42, 6010.5, 6048.35, 6086.84, 6126.03, 6169.05, 6188.01, 6242.23,
6280.41, 6318.05, 6355.37, 6392.51, 6429.85, 6467.74, 6506.39, 6545.78,
6585.83, 6626.48, 6670.72, 6691.27, 6747., 6786.71, 6825.97, 6864.81, 6903.47,
6942.35, 6981.8, 7021.99, 7062.95, 7104.54, 7146.88, 7192.41, 7214.33,
7271.93, 7313.14, 7353.71, 7394.04, 7434.22, 7474.64, 7515.64, 7557.39,
7599.9, 7643.04, 7686.78, 7733.58, 7757.13, 7816.16, 7858.9, 7901.17, 7943.01,
7984.72, 8026.68, 8069.23, 8112.53, 8156.58, 8201.27, 8246.87, 8295.05,
8319.74, 8381.04, 8425.29, 8468.56, 8511.9, 8555.11, 8598.61, 8642.72,
8687.6, 8733.22, 8779.47, 8826.29, 8875.81, 8902.15, 8964.73, 9010.49,
9055.83, 9100.75, 9145.75, 9190.92, 9237.17, 9283.75, 9332.92, 9381.14}
```

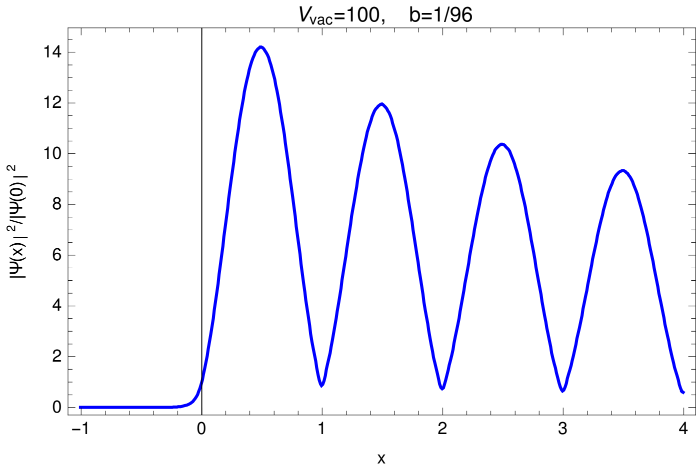
RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

```
In[78]:= xsLeft = 1 + q / 2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
      Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q (in this case Vvac=50 and q=1/6)

In[79]:=
```
RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|^2/|Ψ(0)|^2"}, PlotRange → All,
  PlotLabel → StringJoin[{" Vvac=", ToString[Vvac] , ",     b=", "1/96"}],
  PlotStyle → Blue, Joined → True]
```

Out[79]=



R(x) for Vvac=110

In[80]:=
```
Vvac = 110;
V0Vector[[1]] = Vvac;  V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[82]:=
```
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]
```

Out[82]=
```
{7.06186, 7.10707, 7.24146, 7.45938, 7.7514, 8.10289, 8.4935, 8.89552, 9.27433,
 9.58901, 9.79922, 28.6302, 28.7446, 29.3199, 30.199, 31.3424, 32.6902, 34.1646,
 35.6785, 37.1203, 38.3473, 39.1898, 65.1269, 65.2105, 67.0849, 69.0288,
 71.5056, 74.3389, 77.3885, 80.5139, 83.5419, 86.2127, 88.1398, 112.188,
 112.198, 121.036, 121.743, 122.8, 125.361, 129.088, 133.425, 138.031, 142.621,
 146.709, 149.553, 151.608, 154.175, 156.829, 179.167, 179.182, 194.239,
 197.759, 201.896, 205.856, 209.891, 214.71, 220.423, 226.666, 233.07, 239.235,
 244.443, 255.624, 255.707, 284.738, 287.223, 291.015, 296.404, 303.095,
 310.623, 318.609, 326.792, 334.921, 342.651, 349.396, 354.209, 355.709,
 393.07, 394.699, 400.43, 408.156, 416.989, 426.398, 436.054, 445.68, 454.933,
 463.348, 470.541, 476.597, 481.565, 520.045, 521.401, 530.189, 539.903,
 550.532, 561.588, 572.7, 583.548, 593.781, 603.186, 611.984, 620.552, 628.251,
 666.171, 667.588, 679.78, 691.307, 703.65, 716.24, 728.717, 740.761, 752.156,
 763.009, 773.778, 784.662, 794.719, 831.915, 833.555, 849.21, 862.459,
 876.383, 890.449, 904.262, 917.562, 930.305, 942.806, 955.526, 968.539,
 980.806, 1017.28, 1019.3, 1038.28, 1053.22, 1068.75, 1084.26, 1099.42,
 1114.06, 1128.27, 1142.48, 1157.09, 1172.09, 1186.51, 1222.47, 1224.97,
 1247.17, 1263.76, 1280.79, 1297.73, 1314.26, 1330.29, 1346.04, 1361.95,
 1378.39, 1395.3, 1411.77, 1447.36, 1450.5, 1475.68, 1493.92, 1512.5, 1530.88,
 1548.81, 1566.27, 1583.59, 1601.2, 1619.43, 1638.16, 1656.66, 1692.11,
 1695.97, 1724.04, 1743.88, 1763.93, 1783.74, 1803.07, 1822.02, 1840.91,
 1860.21, 1880.16, 1900.67, 1921.11, 1956.58, 1961.31, 1992.01, 2013.46,
```

```
2035.05, 2056.3, 2077.07, 2097.51, 2118., 2138.96, 2160.61, 2182.86, 2205.21,
2240.91, 2246.57, 2279.84, 2302.87, 2325.9, 2348.59, 2370.81, 2392.76, 2414.84,
2437.45, 2460.77, 2484.73, 2508.88, 2544.94, 2551.67, 2587.28, 2611.88,
2636.45, 2660.6, 2684.29, 2707.76, 2731.43, 2755.67, 2780.65, 2806.28, 2832.25,
2868.84, 2876.67, 2914.59, 2940.75, 2966.75, 2992.35, 3017.52, 3042.52,
3067.77, 3093.63, 3120.24, 3147.52, 3175.21, 3212.41, 3221.48, 3261.5,
3289.22, 3316.76, 3343.83, 3370.49, 3397.02, 3423.85, 3451.32, 3479.56,
3508.47, 3537.9, 3575.86, 3586.16, 3628.3, 3657.56, 3686.52, 3715.06, 3743.2,
3771.27, 3799.69, 3828.76, 3858.6, 3889.12, 3920.19, 3958.97, 3970.63, 4014.68,
4045.49, 4075.99, 4106.01, 4135.66, 4165.27, 4195.26, 4225.92, 4257.36,
4289.49, 4322.25, 4361.96, 4374.94, 4420.98, 4453.31, 4485.22, 4516.72,
4547.87, 4579.02, 4610.58, 4642.83, 4675.85, 4709.57, 4743.91, 4784.59,
4799.03, 4846.82, 4880.69, 4914.18, 4947.16, 4979.82, 5012.52, 5045.64,
5079.47, 5114.07, 5149.37, 5185.38, 5227.12, 5242.93, 5292.63, 5328.01,
5362.89, 5397.36, 5431.53, 5465.77, 5500.46, 5535.86, 5572.03, 5608.91,
5646.44, 5689.25, 5706.59, 5757.94, 5794.86, 5831.32, 5867.29, 5902.98,
5938.76, 5975.01, 6011.98, 6049.72, 6088.16, 6127.35, 6171.33, 6190.07,
6243.29, 6281.71, 6319.54, 6356.99, 6394.19, 6431.51, 6469.32, 6507.86,
6547.16, 6587.16, 6627.83, 6672.96, 6693.29, 6748.07, 6788.02, 6827.47,
6866.43, 6905.15, 6944.01, 6983.38, 7023.47, 7064.34, 7105.89, 7148.25,
7194.63, 7216.32, 7273.01, 7314.47, 7355.21, 7395.66, 7435.89, 7476.29,
7517.21, 7558.87, 7601.29, 7644.4, 7688.17, 7735.76, 7759.08, 7817.26, 7860.24,
7902.67, 7944.64, 7986.4, 8028.33, 8070.8, 8114.01, 8157.99, 8202.63, 8248.28,
8297.23, 8321.67, 8382.14, 8426.64, 8470.08, 8513.53, 8556.78, 8600.26, 8644.3,
8689.08, 8734.63, 8780.86, 8827.73, 8877.98, 8904.07, 8965.86, 9011.86,
9057.36, 9102.39, 9147.48, 9192.63, 9238.95, 9285.46, 9335.17, 9383.42}
```

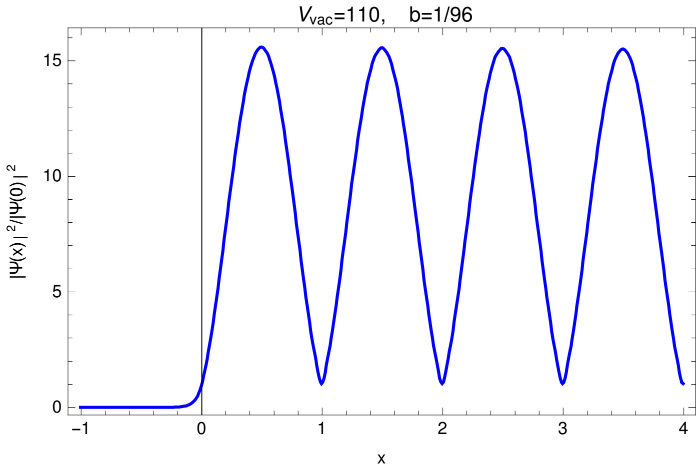
RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

In[83]:=
```
xsLeft = 1 + q / 2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
      Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q   (in this case Vvac=50 and q=1/6)

In[84]:=
```
RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|²/|Ψ(0)|²"}, PlotRange → All,
  PlotLabel → StringJoin[{" Vvac=", ToString[Vvac] , ",     b=", "1/96"}],
  PlotStyle → Blue, Joined → True]
```

Out[84]=



R(x) for Vvac=120

In[85]:=
```
Vvac = 120;
V0Vector[[1]] = Vvac; V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[87]:=
```
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]
```

Out[87]=
```
{7.07002, 7.12415, 7.25908, 7.47614, 7.76665, 8.1161, 8.50424, 8.90348, 9.27943,
 9.59152, 9.79989, 28.6922, 28.8436, 29.391, 30.2645, 31.4017, 32.7416,
 34.2072, 35.7111, 37.1421, 38.3587, 39.193, 65.4692, 65.6068, 67.2085,
 69.1673, 71.6387, 74.461, 77.4962, 80.6036, 83.6089, 86.2521, 88.1522, 115.23,
 115.258, 121.733, 124.643, 128.039, 130.253, 131.566, 134.385, 138.75,
 143.497, 148.215, 152.56, 156.043, 158.482, 158.717, 183.692, 183.723,
 194.51, 198.589, 203.562, 208.543, 212.98, 217.157, 221.95, 227.615, 233.724,
 239.698, 244.668, 260.81, 260.864, 285.384, 289.099, 293.471, 298.514,
 304.623, 311.761, 319.562, 327.705, 335.915, 343.871, 351.012, 358.241,
 358.821, 394.513, 397.283, 402.405, 409.606, 418.148, 427.444, 437.126,
 446.92, 456.535, 465.534, 473.241, 478.909, 482.461, 522.203, 524.36, 531.644,
 541.096, 551.621, 562.696, 573.953, 585.095, 595.756, 605.521, 614.195,
 622.026, 628.769, 668.72, 670.728, 680.965, 692.409, 704.744, 717.432,
 730.124, 742.495, 754.223, 765.164, 775.593, 785.832, 795.171, 834.675,
 836.777, 850.245, 863.521, 877.506, 891.721, 905.781, 919.385, 932.34,
 944.771, 957.114, 969.596, 981.271, 1020.12, 1022.52, 1039.25, 1054.28,
 1069.91, 1085.6, 1101.02, 1115.91, 1130.24, 1144.3, 1158.56, 1173.12, 1187.01,
 1225.34, 1228.16, 1248.1, 1264.82, 1281.99, 1299.13, 1315.9, 1332.14, 1347.94,
 1363.68, 1379.79, 1396.32, 1412.34, 1450.21, 1453.61, 1476.61, 1495., 1513.74,
 1532.32, 1550.48, 1568.11, 1585.43, 1602.86, 1620.79, 1639.19, 1657.29,
 1694.94, 1699., 1724.96, 1744.98, 1765.19, 1785.21, 1804.76, 1823.84, 1842.71,
 1861.82, 1881.5, 1901.73, 1921.82, 1959.35, 1964.24, 1992.94, 2014.58,
```

```
2036.34, 2057.8, 2078.77, 2099.31, 2119.75, 2140.53, 2161.94, 2183.95,
2205.99, 2243.64, 2249.4, 2280.77, 2304., 2327.22, 2350.12, 2372.52, 2394.55,
2416.56, 2438.99, 2462.1, 2485.84, 2509.74, 2547.61, 2554.41, 2588.23,
2613.04, 2637.8, 2662.14, 2686., 2709.53, 2733.13, 2757.2, 2781.98, 2807.42,
2833.17, 2871.46, 2879.31, 2915.55, 2941.93, 2968.11, 2993.91, 3019.23,
3044.27, 3069.45, 3095.15, 3121.58, 3148.69, 3176.2, 3214.98, 3224.03,
3262.48, 3290.42, 3318.14, 3345.4, 3372.19, 3398.76, 3425.51, 3452.83, 3480.9,
3509.66, 3538.95, 3578.38, 3588.63, 3629.29, 3658.77, 3687.92, 3716.64,
3744.9, 3773., 3801.33, 3830.26, 3859.94, 3890.34, 3921.29, 3961.44, 3973.02,
4015.69, 4046.72, 4077.41, 4107.6, 4137.36, 4166.98, 4196.89, 4227.42,
4258.71, 4290.72, 4323.4, 4364.39, 4377.26, 4421.99, 4454.55, 4486.66,
4518.31, 4549.57, 4580.73, 4612.2, 4644.32, 4677.21, 4710.83, 4745.1, 4786.97,
4801.28, 4847.86, 4881.96, 4915.62, 4948.76, 4981.51, 5014.21, 5047.26,
5080.96, 5115.44, 5150.65, 5186.61, 5229.46, 5245.13, 5293.68, 5329.29,
5364.34, 5398.96, 5433.22, 5467.45, 5502.06, 5537.35, 5573.41, 5610.2, 5647.7,
5691.55, 5708.74, 5759.01, 5796.15, 5832.79, 5868.9, 5904.66, 5940.43,
5976.61, 6013.46, 6051.1, 6089.47, 6128.64, 6173.61, 6192.17, 6244.36,
6283.01, 6321.01, 6358.6, 6395.87, 6433.18, 6470.92, 6509.35, 6548.55,
6588.49, 6629.15, 6675.2, 6695.34, 6749.16, 6789.34, 6828.95, 6868.04,
6906.82, 6945.67, 6984.97, 7024.95, 7065.73, 7107.22, 7149.59, 7196.85,
7218.34, 7274.11, 7315.79, 7356.7, 7397.27, 7437.57, 7477.95, 7518.8, 7560.36,
7602.69, 7645.75, 7689.53, 7737.95, 7761.07, 7818.38, 7861.58, 7904.17,
7946.25, 7988.07, 8029.99, 8072.39, 8115.5, 8159.39, 8203.99, 8249.66,
8299.41, 8323.64, 8383.25, 8427.98, 8471.59, 8515.15, 8558.45, 8601.92,
8645.88, 8690.58, 8736.05, 8782.24, 8829.14, 8880.16, 8906.02, 8967., 9013.22,
9058.88, 9104.02, 9149.2, 9194.35, 9240.75, 9287.19, 9337.55, 9385.81}
```

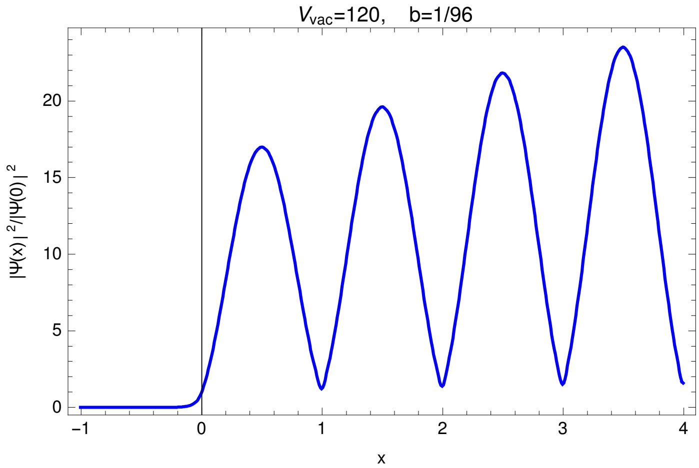
RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

In[88]:=
```
xsLeft = 1 + q / 2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
     Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q (in this case Vvac=50 and q=1/6)

In[89]:=
```
RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|²/|Ψ(0)|²"}, PlotRange → All,
  PlotLabel → StringJoin[{" Vvac=", ToString[Vvac] , ",     b=", "1/96"}],
  PlotStyle → Blue, Joined → True]
```

Out[89]=



R(x) for Vvac=150

In[90]:=
```
Vvac = 150;
V0Vector[[1]] = Vvac;  V0Vector[[Length[xrVector]]] = Vvac;
```

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

In[92]:=
```
Energies = EnV[Nterms, L, V0Vector, xrVector, bVector]
```

Out[92]=
```
{7.08309, 7.15689, 7.30016, 7.51846, 7.80653, 8.15128, 8.53311, 8.92496, 9.29322,
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8695.13, 8740.33, 8786.35, 8833.24, 8886.69, 8912.1, 8970.53, 9017.28,
9063.37, 9108.85, 9154.32, 9199.5, 9246.21, 9292.45, 9345.45, 9393.76}
```

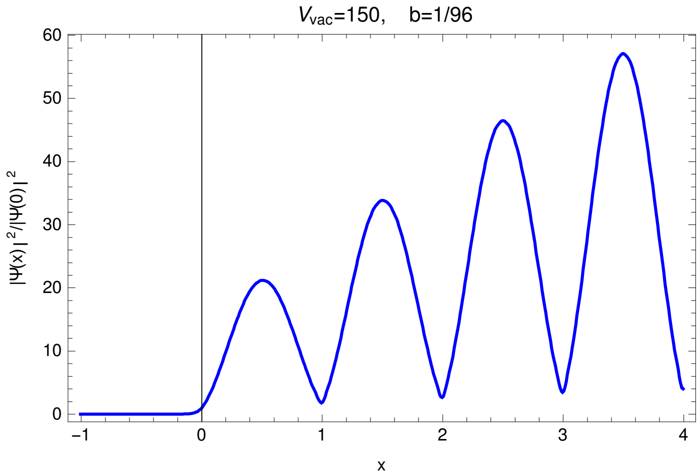
RxVector is a table of {x,R(x)} with x=0.01, 0.02,...,5

In[93]:=
```
xsLeft = 1 + q/2;
fp1 = ProbDensity[1, xsLeft, Nterms, Nterms, L, V0Vector, xrVector, bVector ];
RxVector = Table[{x - xsLeft, ProbDensity[1, x, Nterms,
      Nterms, L, V0Vector, xrVector, bVector ] / fp1}, {x, 0, 5, 0.01}];
```

RxPlot[Vvac,q] is the plot of R(x) for the case with V_{vac} =Vvac and b=q (in this case Vvac=50 and q=1/6)

In[94]:=
```
RxPlot[Vvac, q] = ListPlot[RxVector, Frame → True,
  FrameLabel -> {"x", "|Ψ(x)|^2/|Ψ(0)|^2"}, PlotRange → All,
  PlotLabel → StringJoin[{" Vvac=", ToString[Vvac] , ",      b=", "1/96"}],
  PlotStyle → Blue, Joined → True]
```

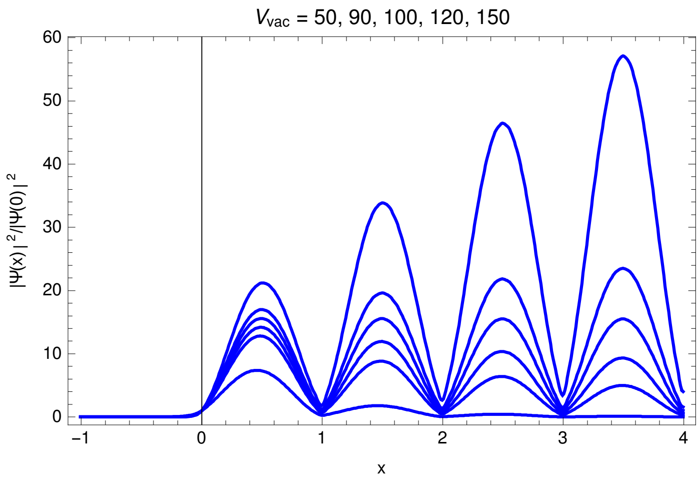
Out[94]=



Comparison of R(x) for several value of V_{vac}

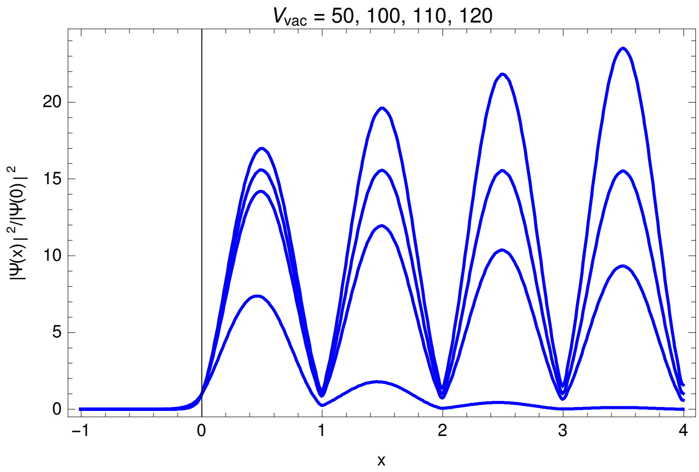
In[95]:=
```
Show[{RxPlot[50, q], RxPlot[90, q], RxPlot[100, q],
  RxPlot[110, q], RxPlot[120, q], RxPlot[150, q]}, PlotRange → All,
 PlotLabel → StringJoin[{"Vvac = 50, 90, 100, 120, 150"}]]
```

Out[95]=



In[96]:=
```
Show[{RxPlot[50, q], RxPlot[100, q], RxPlot[110, q], RxPlot[120, q]},
  PlotRange → All, PlotLabel → StringJoin[{"Vvac = 50, 100, 110, 120"}]]
```

Out[96]=



In[97]:=
```
Show[{RxPlot[50, q], RxPlot[100, q], RxPlot[120, q]},
  PlotRange → All, PlotLabel → StringJoin[{"Vvac = 50, 100, 120"}]]
```

Out[97]=