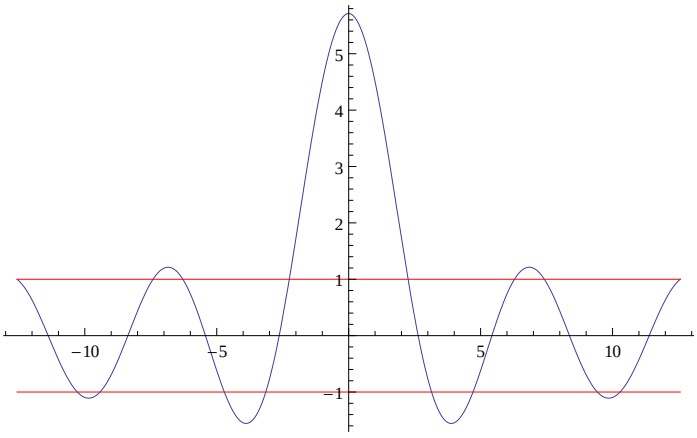
Kronig - Penney Model

```
r = p → 3 π / 2;

f[Ka_] = p / Ka Sin[Ka] + Cos[Ka];

p1 = Plot[f[Ka] /. r, {Ka, -4 π, 4 π}];

p2 = Plot[{1, -1}, {Ka, -4 π, 4 π}, PlotStyle → RGBColor[1, 0, 0]];

Show[p1, p2]
```



- **ka = 0**

```
FindRoot[(p / Ka Sin[Ka] + Cos[Ka] /. r) == 1, {Ka, π}]
```

{Ka → 2.2505}

- **ka = π**

```
FindRoot[(p / Ka Sin[Ka] + Cos[Ka] /. r) == -1, {Ka, π}]
```

{Ka → 3.14159}

- **ka = π**

```
FindRoot[(p / Ka Sin[Ka] + Cos[Ka] /. r) == -1, {Ka, 1.5 π}]
```

{Ka → 4.71239}

- **ka = 2π**

```
FindRoot[(p / Ka Sin[Ka] + Cos[Ka] /. r) == 1, {Ka, 2 π}]
```

{Ka → 6.28319}

- **ka = 2π**

```
FindRoot[(p / Ka Sin[Ka] + Cos[Ka] /. r) == 1, {Ka, 2.5 π}]
```

{Ka → 7.4154}

- **ka = 3π**

```
FindRoot[(p / Ka Sin[Ka] + Cos[Ka] /. r) == -1, {Ka, 3 π}]
```

{Ka → 9.42478}

- **ka = 3π**

```
FindRoot[(p/Ka Sin[Ka] + Cos[Ka] /. r) == -1, {Ka, 3.5π}]
```

```
{Ka → 10.2841}
```

- **ka = 4π**

```
FindRoot[(p/Ka Sin[Ka] + Cos[Ka] /. r) == +1, {Ka, 4π}]
```

```
{Ka → 12.5664}
```

```
ϵ[Ka_] = (Ka/π)^2;
```

- **Energy bands and gaps - first approximation (gaps are correct, but lines not straight)**

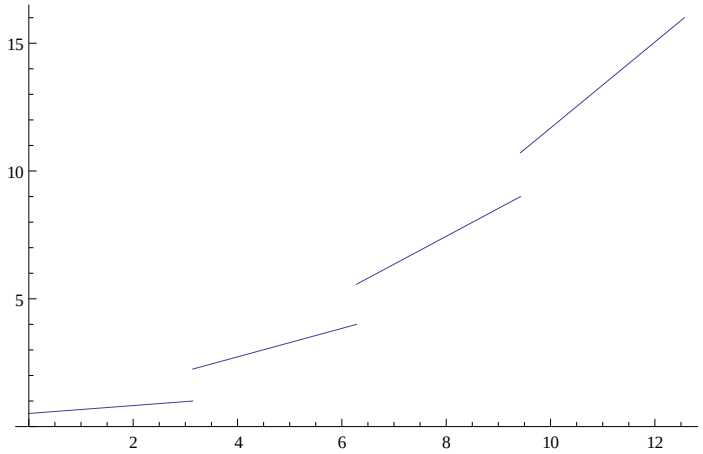
```
p1 = ListPlot[{{0, ϵ[2.25050361356163]}, {π, ϵ[π]}}, Joined→ True];
```

```
p2 = ListPlot[{{π, ϵ[4.71238898038469]}, {2π, ϵ[2π]}}, Joined→ True];
```

```
p3 = ListPlot[{{2π, ϵ[7.41539561136493]}, {3π, ϵ[3π]}}, Joined→ True];
```

```
p4 = ListPlot[{{3π, ϵ[10.2841154507764]}, {4π, ϵ[4π]}}, Joined→ True];
```

```
f1 = Show[p1, p2, p3, p4, PlotRange→ All]
```



- **Energy bands and gaps - correct**

```
table1 = Table[{ka,
    (FindRoot[(p/Ka Sin[Ka] + Cos[Ka] /. r) == Cos[ka], {Ka, 0.5π}])[[1, 2]]
  }, {ka, 0, π, π/20}]; table1// TableForm;
```

```
e1 = Interpolation[table1];
```

```
pc1 = Plot[ϵ[e1[ka]], {ka, 0, π}, PlotStyle→ RGBColor[1, 0, 0]];
```

```
table2 = Table[{ka,
    (FindRoot[(p/Ka Sin[Ka] + Cos[Ka] /. r) == Cos[ka], {Ka, 1.5π}])[[1, 2]]
  }, {ka, π, 2π, π/20}]; table2// TableForm;
```

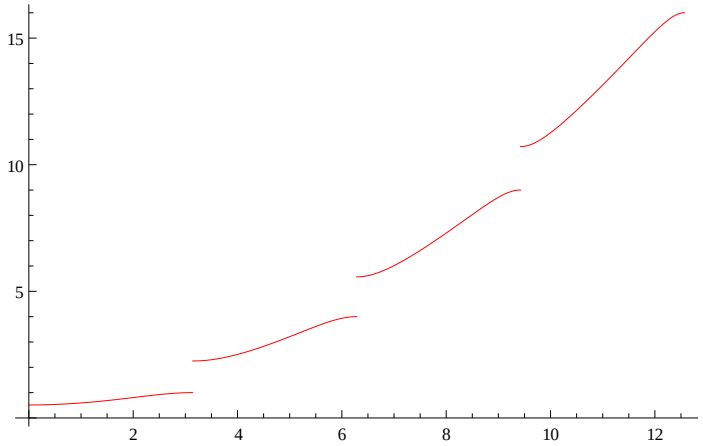
```
e2 = Interpolation[table2];
```

```
pc2 = Plot[ϵ[e2[ka]], {ka, π, 2π}, PlotStyle→ RGBColor[1, 0, 0]];
```

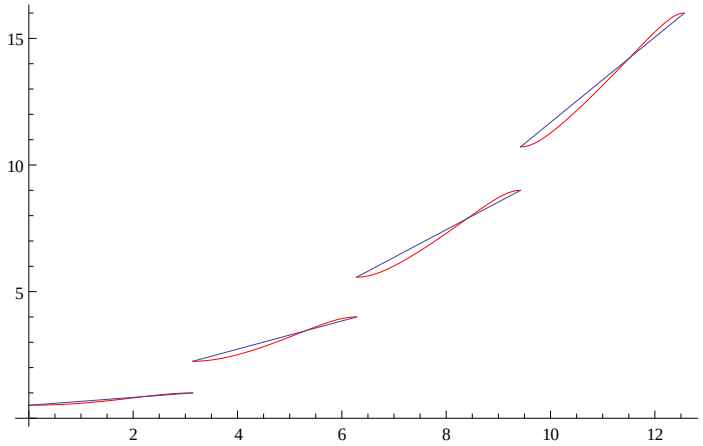
```
table3 = Table[{ka,
    (FindRoot[(p/Ka Sin[Ka] + Cos[Ka] /. r) == Cos[ka], {Ka, 2.5π}])[[1, 2]]
  }, {ka, 2π, 3π, π/20}]; table3// TableForm;
```

```
e3 = Interpolation[table3];
```

```
pc3 = Plot[ϵ[e3[ka]], {ka, 2π, 3π}, PlotStyle→ RGBColor[1, 0, 0]];

table4 = Table[{ka,
    (FindRoot[(p/Ka Sin[Ka] + Cos[Ka] /. r) == Cos[ka], {Ka, 3.5π}])[[1, 2]]
  }, {ka, 3π, 4π, π/20}]; table4 // TableForm;

e4 = Interpolation[table4];

pc4 = Plot[ϵ[e4[ka]], {ka, 3π, 4π}, PlotStyle→ RGBColor[1, 0, 0]];

Show[pc1, pc2, pc3, pc4, PlotRange→ All, AxesOrigin→ {0, 0}]
```




```
Show[pc1, pc2, pc3, pc4, f1, PlotRange→ All, AxesOrigin→ {0, 0}]
```



```
Show[p1, pc1, PlotRange→ All, AxesOrigin→ {0, 0}]
```