WKB wavefunctions for simple harmonics

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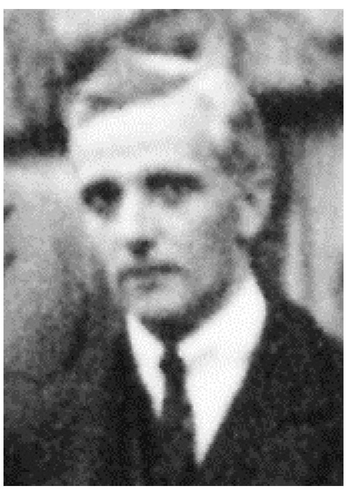
Gregor Wentzel (February 17, 1898, in Düsseldorf, Germany – August 12, 1978, in Ascona, Switzerland) was a German physicist known for development of quantum mechanics. Wentzel, Hendrik Kramers, and Léon Brillouin developed the Wentzel–Kramers–Brillouin approximation in 1926. In his early years, he contributed to X-ray spectroscopy, but then broadened out to make contributions to quantum mechanics, quantum electrodynamics, and meson theory.
http://en.wikipedia.org/wiki/Gregor_Wentzel

Hendrik Anthony "Hans" Kramers (Rotterdam, February 2, 1894 – Oegstgeest, April 24, 1952) was a Dutch physicist.
http://en.wikipedia.org/wiki/Hendrik_Anthony_Kramers

Léon Nicolas Brillouin (August 7, 1889 – October 4, 1969) was a French physicist. He made contributions to quantum mechanics, radio wave propagation in the atmosphere, solid state physics, and information theory.



http://en.wikipedia.org/wiki/L%C3%A9on_Brillouin

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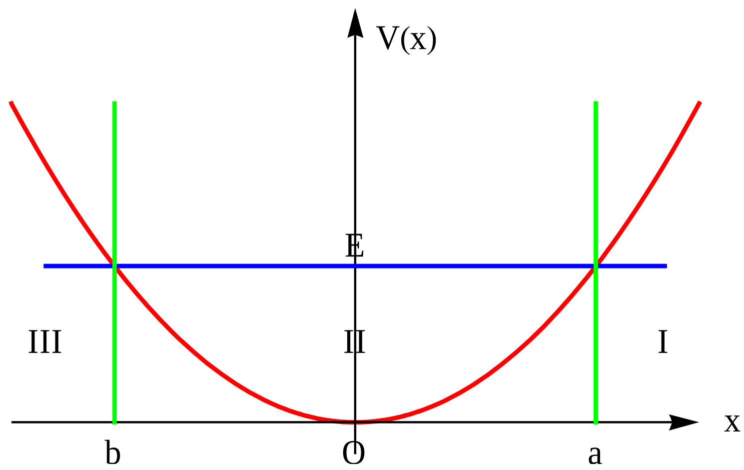
1. Determination of wave functions using the WKB Approximation

In order to determine the eave function of the simple harmonics, we use the connection formula of the WKB approximation.



The potential energy is expressed by

$$V(x) = \frac{1}{2} m\omega_0{}^2 x^2 .$$

The x-coordinates a and b (the classical turning points) are obtained as

$$a = \sqrt{\frac{2\varepsilon}{m\omega_0{}^2}} , \qquad b = -\sqrt{\frac{2\varepsilon}{m\omega_0{}^2}} ,$$

from the equation

$$\varepsilon = V(x) = \frac{1}{2} m\omega_0{}^2 x^2 ,$$

or

$$\varepsilon = \frac{1}{2} m\omega_0{}^2 a^2 = \frac{1}{2} m\omega_0{}^2 b^2 ,$$

where ε is the constant total energy. Here we apply the connection formula (I, upward) at $x = a$.

Connection formula-I (upward):

$$\psi_{II} = \frac{2A}{\sqrt{k(x)}}\cos(\int_x^a k(x)dx - \frac{\pi}{4}) - \frac{B}{\sqrt{k(x)}}\sin(\int_x^a k(x)dx - \frac{\pi}{4})]$$

$\Rightarrow$

$$\psi_I = \frac{A}{\sqrt{\kappa(x)}}\exp(-\int_a^x \kappa(x)dx) + \frac{B}{\sqrt{\kappa(x)}}\exp(\int_a^x \kappa(x)dx)]$$

In ψ_I , B should be equal to zero: $B = 0$. Then we have

$$\psi_I = \frac{A}{\sqrt{\kappa(x)}}\exp(-\int_a^x \kappa(x)dx),$$

for $x>b$. The wave function ψ_{II} is obtained as

$$\begin{aligned}
\psi_{II} &= \frac{2A}{\sqrt{k(x)}}\cos(\int_x^a k(x)dx - \frac{\pi}{4}) \\
&= \frac{2A}{\sqrt{k(x)}}\cos(\int_x^b k(x)dx + \int_b^a k(x)dx - \frac{\pi}{4}) \\
&= \frac{2A}{\sqrt{k(x)}}\cos(-\int_b^x k(x)dx + \int_b^a k(x)dx - \frac{\pi}{2} + \frac{\pi}{4}) \\
&= \frac{2A}{\sqrt{k(x)}}\sin\{\int_b^a k(x)dx - [\int_b^x k(x)dx - \frac{\pi}{4}]\} \\
&= \frac{2A}{\sqrt{k(x)}}[\sin(\int_b^a k(x)dx)\cos(\int_b^x k(x)dx - \frac{\pi}{4}) - \cos(\int_b^a k(x)dx)\sin(\int_b^x k(x)dx - \frac{\pi}{4})]
\end{aligned}$$

Next we use the connection formula (II, downward) at $x = b$.

Connection formula-II

$$\psi_{III} = \frac{C}{2\sqrt{\kappa(x)}}\exp(-\int_x^b \kappa(x)dx) + \frac{D}{2\sqrt{\kappa(x)}}\exp(\int_x^b \kappa(x)dx)]$$

$$\Rightarrow$$

$$\psi_{II} = \frac{C}{\sqrt{k(x)}}\cos(\int_b^x k(x)dx - \frac{\pi}{4}) - \frac{D}{2\sqrt{k(x)}}\sin(\int_b^x k(x)dx - \frac{\pi}{4})]$$

The comparison of this equation with

$$\psi_{II} = \frac{2A}{\sqrt{k(x)}}\sin(\int_b^a k(x)dx)\cos(\int_b^x k(x)dx - \frac{\pi}{4}) - \frac{2A}{\sqrt{k(x)}}\cos(\int_b^a k(x)dx)\sin(\int_b^x k(x)dx - \frac{\pi}{4})],$$

yields the relation between *C*, *D*, and *A*,

$$C = \frac{2A}{\sqrt{k(x)}}\sin(\int_b^a k(x)dx), \qquad \text{and} \qquad D = 4A\cos(\int_b^a k(x)dx),$$

In ψ_{III}, *D* should be equal to zero: *D* = 0. This means that

$$D = 4A\cos(\int_b^a k(x)dx) = 0, \qquad \cos(\int_b^a k(x)dx) = 0,$$

or

$$\int_b^a k(x)dx = (n + \frac{1}{2})\pi,$$

where *n* is a positive integer. This integral can be calculated as

$$\int_b^a k(x)dx = \frac{\sqrt{2m}}{\hbar}\int_{-a}^{a}\sqrt{\frac{1}{2}m\omega_0{}^2(a^2-x^2)}dx$$
$$= \frac{m\omega_0}{\hbar}\int_{-a}^{a}\sqrt{a^2-x^2}dx$$
$$= \frac{m\omega_0}{\hbar}\frac{\pi a^2}{2} = (n+\frac{1}{2})\pi$$

which means that

$$\varepsilon = \frac{1}{2}m\omega_0{}^2a^2 = \frac{1}{2}m\omega_0{}^2\frac{2\hbar}{\pi m\omega_0}(n+\frac{1}{2})\pi = \hbar\omega_0(n+\frac{1}{2})$$

In other words, the energy is quantized. This is amazing. Noting that

$$\sin[\int_b^a k(x)dx] = \sin[(n+\frac{1}{2})\pi] = \cos(n\pi) = (-1)^n,$$

we have the final forms of the wave functions

$$\psi_{III} = \frac{A}{\sqrt{k(x)}}\sin(\int_b^a k(x)dx)\exp(-\int_x^b \kappa(x)dx)$$
$$= \frac{A(-1)^n}{\sqrt{k(x)}}\exp(-\int_x^b \kappa(x)dx)$$

for $x<b$ and

$$\psi_{II} = \frac{2A}{\sqrt{k(x)}}\sin(\int_b^a k(x)dx)\cos(\int_b^x k(x)dx - \frac{\pi}{4})$$
$$= \frac{2A(-1)^n}{\sqrt{k(x)}}\cos(\int_b^x k(x)dx - \frac{\pi}{4})$$

for $b<x<a$.

2. WKB wave functions for simple harmonics

We introduce a new variable ξ (dimensionless) as,

$$\xi = \beta x,$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}}.$$

The parameters *a* and *b* are rewritten as

$$a = \sqrt{\frac{2\varepsilon}{m\omega_0{}^2}} = \sqrt{\frac{2(n+\frac{1}{2})\hbar\omega_0}{m\omega_0{}^2}} = \sqrt{\frac{(2n+1)\hbar}{m\omega_0}} = \frac{\sqrt{2n+1}}{\beta},$$

and

$$b = -\frac{\sqrt{2n+1}}{\beta}.$$

We also note that $\kappa(x)$ and $k(x)$ are expressed by

$$\begin{aligned}\kappa(x) &= \frac{\sqrt{2m}}{\hbar}\sqrt{V(x) - \hbar\omega_0(n+\frac{1}{2})} \\ &= \frac{\sqrt{2m}}{\hbar}\sqrt{\frac{1}{2}m\omega_0{}^2 x^2 - \hbar\omega_0(n+\frac{1}{2})} \\ &= \beta\sqrt{\xi^2 - (2n+1)}\end{aligned}$$

$$
\begin{aligned}
k(x) &= \frac{\sqrt{2m}}{\hbar}\sqrt{\hbar\omega_0(n+\frac{1}{2})-V(x)} \\
&= \frac{\sqrt{2m}}{\hbar}\sqrt{\hbar\omega_0(n+\frac{1}{2})-\frac{1}{2}m\omega_0{}^2x^2} \\
&= \beta\sqrt{(2n+1)-\xi^2}
\end{aligned}
$$

Using these parameters, we have

$$\int_a^x \kappa(x)dx = \int_{\sqrt{2n+1}}^{\xi}\sqrt{s^2-(2n+1)}ds\,,$$

$$\int_b^x k(x)dx = \int_{-\sqrt{2n+1}}^{\xi}\sqrt{s^2-(2n+1)}ds\,.$$

The wavefunction in the region II;

$$
\begin{aligned}
\psi_{II} &= \frac{2A(-1)^n}{\sqrt{k(x)}}\cos(\int_b^x k(x)dx-\frac{\pi}{4}) \\
&= \frac{A}{\sqrt{\beta}}\frac{2(-1)^n}{[(2n+1)-\xi^2]^{1/4}}\cos[\int_{-\sqrt{2n+1}}^{\xi}\sqrt{s^2-(2n+1)}ds-\frac{\pi}{4}]
\end{aligned}
$$

The wavefunction in the region I

$$
\begin{aligned}
\psi_I &= \frac{A}{\sqrt{\kappa(x)}}\exp[-\int_a^x \kappa(x)dx] \\
&= \frac{A}{\sqrt{\beta}}\frac{1}{[\xi^2-(2n+1)]^{1/4}}\exp[-\int_{\sqrt{2n+1}}^{\xi}\sqrt{s^2-(2n+1)}ds]
\end{aligned}
$$

The wavefunction in the region III

$$\psi_{III} = \frac{A(-1)^n}{\sqrt{\kappa(x)}} \exp[-\int_x^b \kappa(x)dx]$$

$$= \frac{A}{\sqrt{\beta}} \frac{(-1)^n}{[\xi^2-(2n+1)]^{1/4}} \exp[-\int_\xi^{-\sqrt{2n+1}} \sqrt{s^2-(2n+1)}ds]$$

We assume that the parameter $A/\sqrt{\beta}$ is determined from the normalization condition of the wave function.

3. Result from Mathematica: $\psi_n(\xi)$

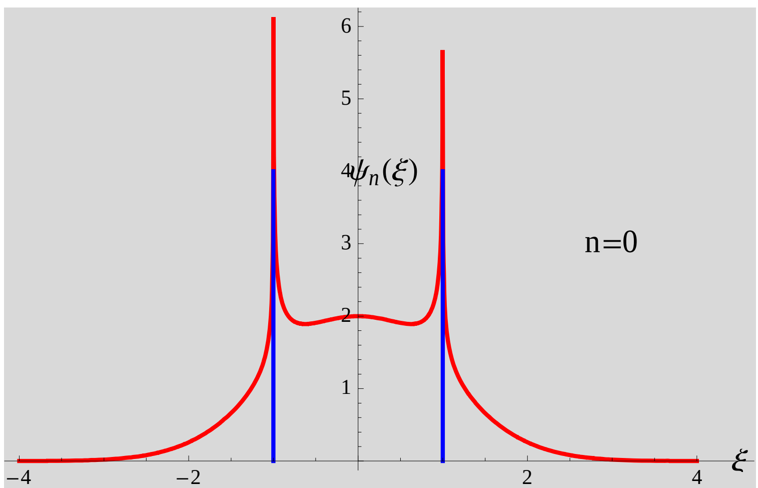


Fig. $n = 0$ (ground state). The blue lines are classical turning points.

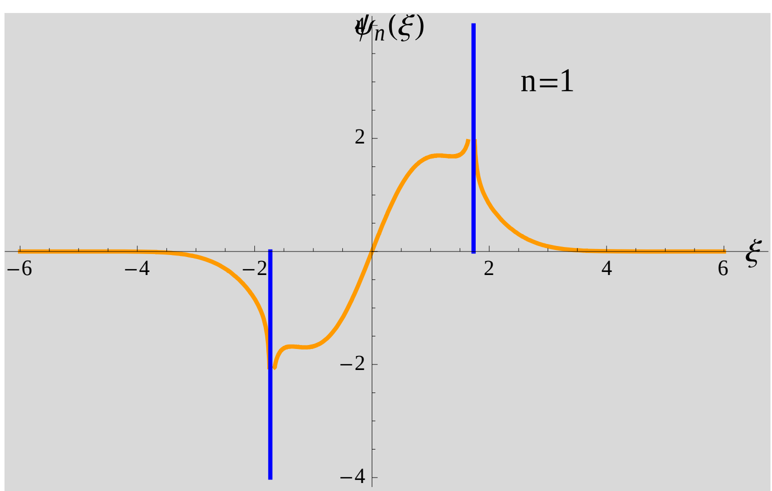


Fig. n = 1. The blue lines are classical turning points.

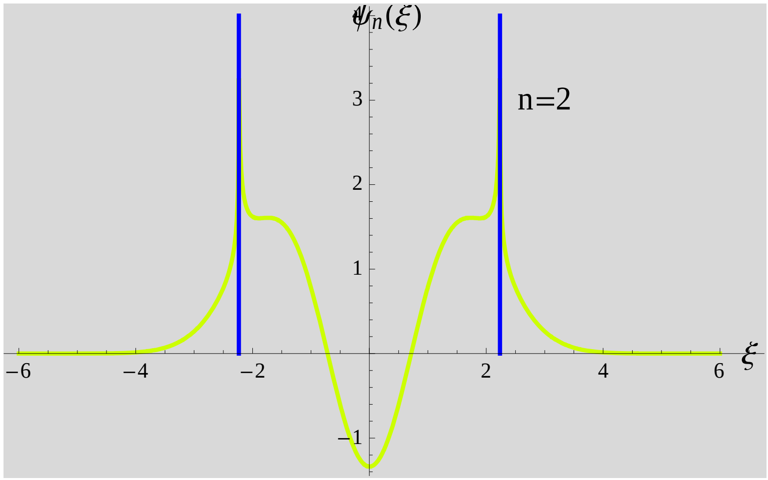


Fig. n = 2. The blue lines are classical turning points.

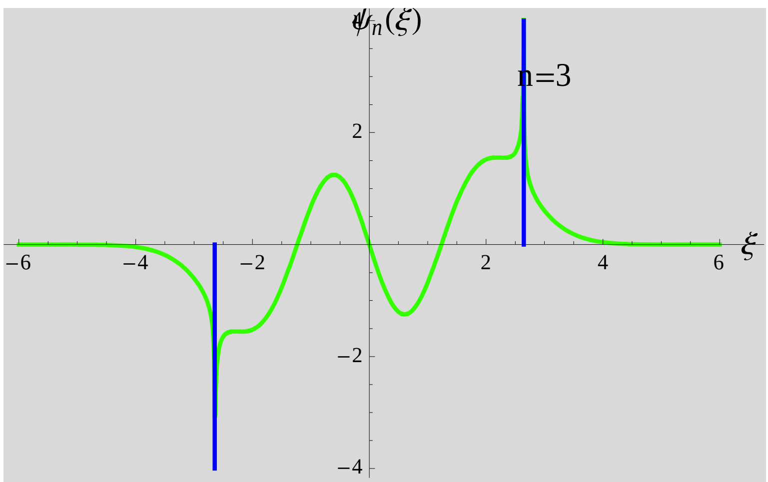


Fig. n = 3. The blue lines are classical turning points.

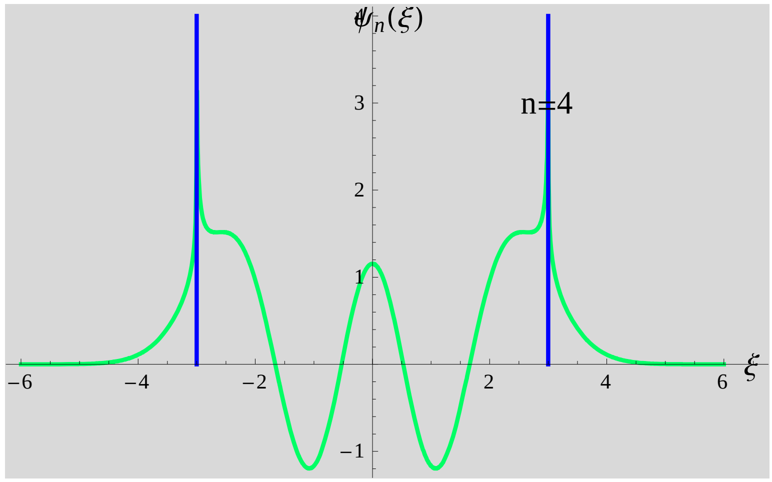


Fig. *n* = 4. The blue lines are classical turning points.

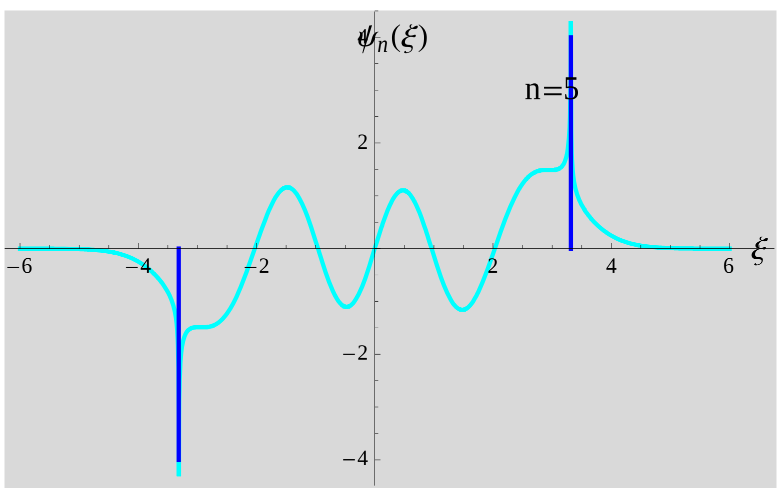


Fig. *n* = 5. The blue lines are classical turning points.

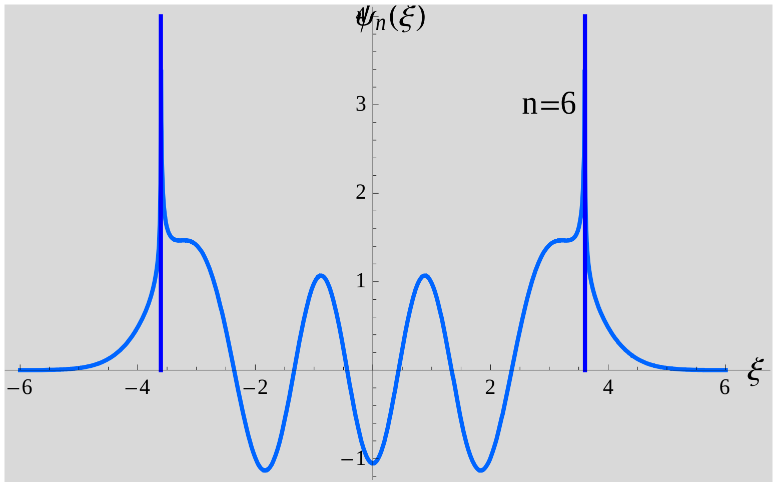
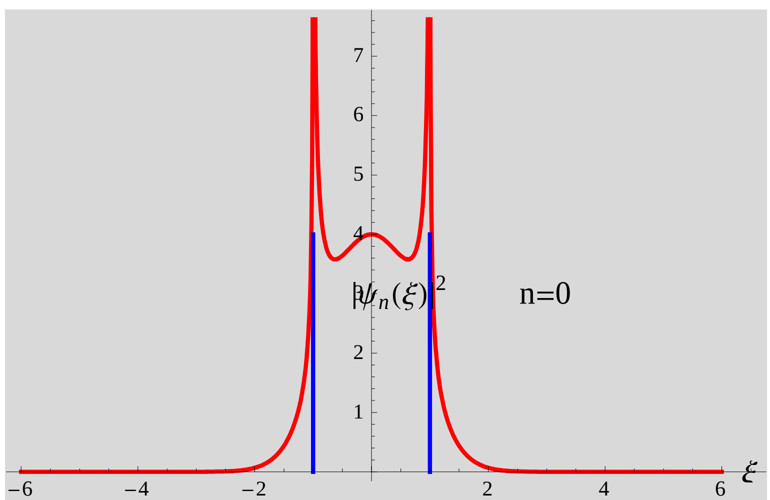
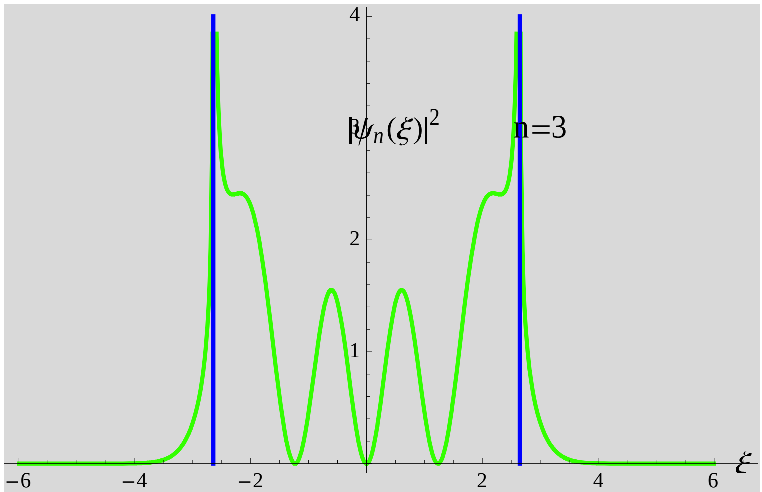


Fig. n = 6. The blue lines are classical turning points.

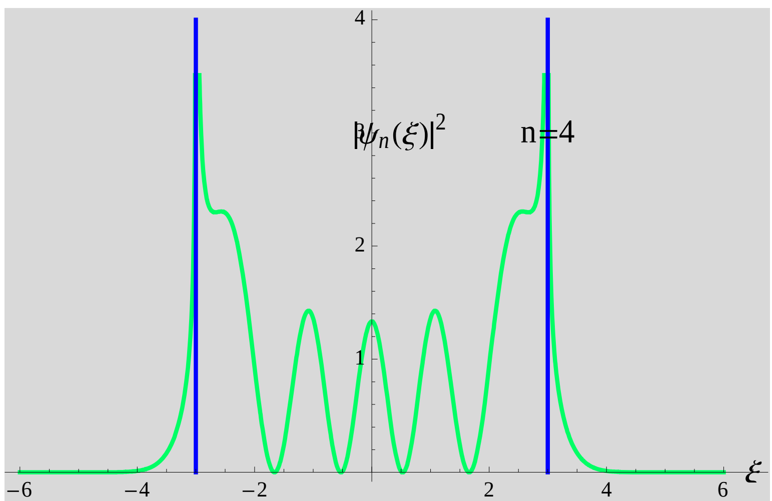
In summary; we see that the WKB solution agrees well with the solutions from the quantum mechanics

4. Result from Mathematica: $|\psi_n(\xi)|^2$

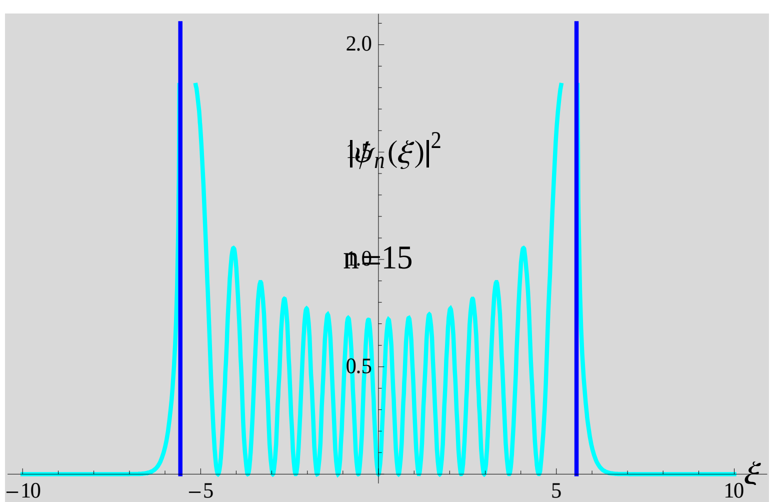




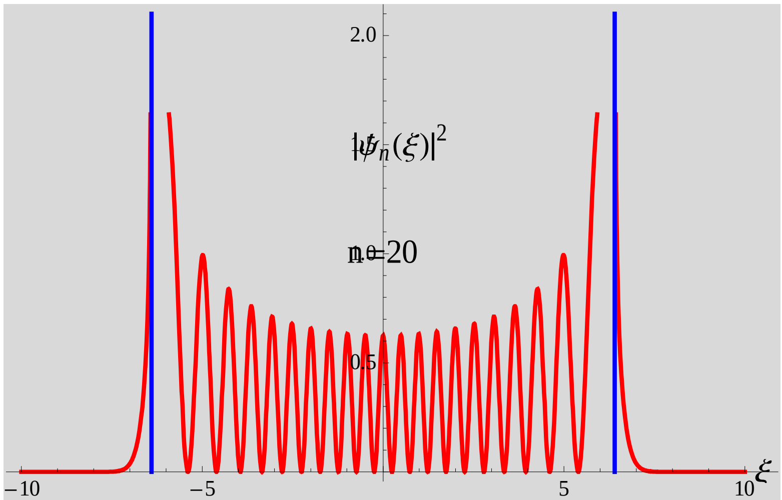
$|\psi_n(\xi)|^2$
n=3
ξ



$|\psi_n(\xi)|^2$
n=4
ξ



$|\psi_n(\xi)|^2$
n=15
ξ



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1. David J. Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, Englewood Cliff, NJ, 1995).
2. David. Bohm, *Quantum Theory* (Dover Publication, Inc, New York, 1979).
3. Eugen Merzbacher, Quantum Mechanics, 3rd edition (John Wiley & Sons, New York, 1998).
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5. Richard L. Liboff, *Introductory Quantum Mechanics*, 4th edition (Addison Wesley, 2002).

APPENDIX-1: Mathematica program

We calculate the following integrals separately,
since it takes a quite long time to calculate. Here we use the results.

```
g3 = Integrate[Sqrt[s^2 - (2 n1 + 1)], {s, ξ1, -Sqrt[2 n1 + 1]}] //
  Simplify[#, {n1 > 0, ξ1 < -Sqrt[2 n1 + 1]}] &;
g1 = Integrate[Sqrt[s^2 - (2 n1 + 1)], {s, Sqrt[2 n1 + 1], ξ1}] //
  Simplify[#, {n1 > 0, ξ1 > Sqrt[2 n1 + 1]}] &;
g2 = Integrate[Sqrt[(2 n1 + 1) - s^2], {s, -Sqrt[2 n1 + 1], ξ1}] //
  Simplify[#, {n1 > 0, -Sqrt[2 n1 + 1] < ξ1 < Sqrt[2 n1 + 1]}] &;
```

$$\text{g11} = \frac{1}{4}\left(2\,\xi 1\sqrt{-1-2\,\text{n1}+\xi 1^2} + (1+2\,\text{n1})\left(\text{Log}[1+2\,\text{n1}] - 2\,\text{Log}\left[\xi 1 + \sqrt{-1-2\,\text{n1}+\xi 1^2}\right]\right)\right);$$

$$\text{g21} = \frac{1}{4}\left(\pi + 2\,\text{n1}\,\pi + 2\,\xi 1\sqrt{1+2\,\text{n1}-\xi 1^2} + (2+4\,\text{n1})\,\text{ArcTan}\left[\frac{\xi 1}{\sqrt{1+2\,\text{n1}-\xi 1^2}}\right]\right);$$

$$\text{g31} = \frac{1}{2}\left(-\xi 1\sqrt{-1-2\,\text{n1}+\xi 1^2} - (1+2\,\text{n1})\,\text{Log}\left[-\sqrt{1+2\,\text{n1}}\right] + (1+2\,\text{n1})\,\text{Log}\left[\xi 1 + \sqrt{-1-2\,\text{n1}+\xi 1^2}\right]\right);$$

$$\psi 1 = \frac{1}{\sqrt{\sqrt{\xi 1^2 - (2\,\text{n1}+1)}}}\,\text{Exp}[-\text{g11}];$$

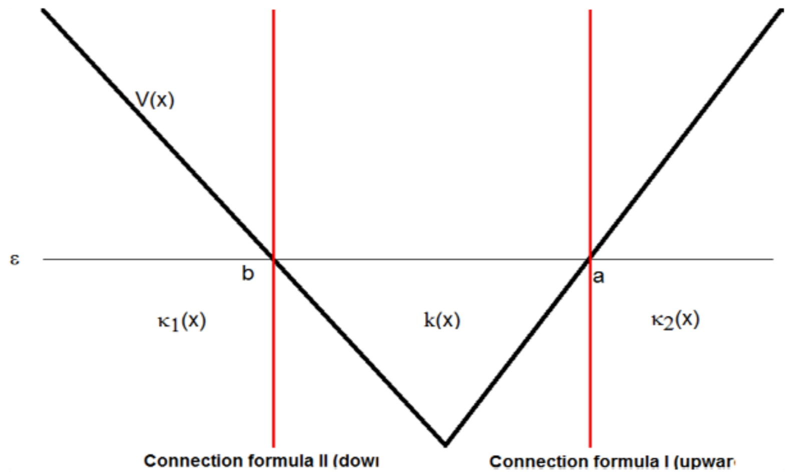
$$\psi 3 = \frac{(-1)^{\text{n1}}}{\sqrt{\sqrt{\xi 1^2 - (2\,\text{n1}+1)}}}\,\text{Exp}[-\text{g31}];$$

$$\psi 2 = \frac{2\,(-1)^{\text{n1}}}{\sqrt{\sqrt{-\xi 1^2 + (2\,\text{n1}+1)}}}\,\text{Cos}\left[\text{g21} - \frac{\pi}{4}\right];$$

```
ψ[n_, ξ_] :=
  (ψ3 UnitStep[-ξ1 - √(2 n1 + 1)] +
      ψ2 (UnitStep[ξ1 + √(2 n1 + 1)] - UnitStep[ξ1 - √(2 n1 + 1)]) +
      ψ1 UnitStep[ξ1 - √(2 n1 + 1)]) /. {n1 → n, ξ1 → ξ} // Simplify;

P[n_, s_] := Module[{h1, h2, h3, n1}, n1 = n;
   h1 = Plot[ψ[n1, ξ], {ξ, -s, s}, PlotStyle → {Hue[0.1 n1], Thick},
     Background → LightGray];
   h2 = Graphics[{Blue, Thick, Line[{{-√(2 n1 + 1), 0}, {-√(2 n1 + 1), (-1)^n1 4}}],
      Line[{{√(2 n1 + 1), 0}, {√(2 n1 + 1), 4}}],
      Text[Style["ξ", Black, 15], {s + 0.5, 0}],
      Text[Style["ψn(ξ)", Black, 15], {0.3, 4}],
      Text[Style[ "n=" <> ToString[n1], Black, 15], {3, 3}]}];
   h3 = Show[h1, h2, PlotRange → All] ];
Q[n_, s_] := Module[{h1, h2, h3, n1}, n1 = n;
   h1 = Plot[ψ[n1, ξ]^2, {ξ, -s, s}, PlotStyle → {Hue[0.1 n1], Thick},
     Background → LightGray];
   h2 = Graphics[{Blue, Thick, Line[{{-√(2 n1 + 1), 0}, {-√(2 n1 + 1), 4}}],
      Line[{{√(2 n1 + 1), 0}, {√(2 n1 + 1), 4}}],
      Text[Style["ξ", Black, 15], {s + 0.5, 0}],
      Text[Style["|ψn(ξ)|^2", Black, 15], {0.5, 3}],
      Text[Style[ "n=" <> ToString[n1], Black, 15], {3, 3}]}];
   h3 = Show[h1, h2, PlotRange → All] ];
```

APPENDIX-2: Connection formula



$$\frac{C}{2\sqrt{\kappa(x)}}\exp(-\int_x^b \kappa(x)dx)+\frac{D}{2\sqrt{\kappa(x)}}\exp(\int_x^b \kappa(x)dx)]$$

$\Rightarrow$

$$\frac{C}{\sqrt{k(x)}}\cos(\int_b^x k(x)dx-\frac{\pi}{4})-\frac{D}{2\sqrt{k(x)}}\sin(\int_b^x k(x)dx-\frac{\pi}{4})]$$

$$\frac{2A}{\sqrt{k(x)}}\cos(\int_x^a k(x)dx-\frac{\pi}{4})-\frac{B}{\sqrt{k(x)}}\sin(\int_x^a k(x)dx-\frac{\pi}{4})$$

$\Rightarrow$

$$\frac{A}{\sqrt{\kappa(x)}}\exp(-\int_a^x \kappa(x)dx)+\frac{B}{\sqrt{\kappa(x)}}\exp(\int_a^x \kappa(x)dx)]$$