WKB wavefunctions for simple harmonics

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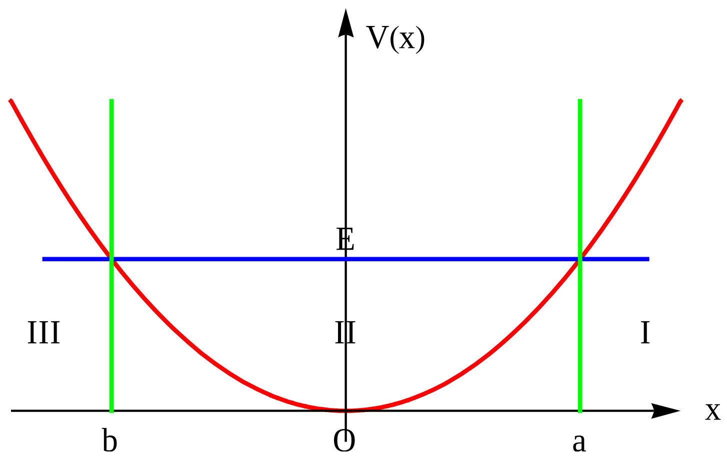
1. Determination of wave functions using the WKB Approximation

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

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

$$= \frac{2A}{\sqrt{k(x)}}\cos(\int_x^b k(x)dx + \int_b^a k(x)dx - \frac{\pi}{4})$$

$$= \frac{2A}{\sqrt{k(x)}}\cos(-\int_b^x k(x)dx + \int_b^a k(x)dx - \frac{\pi}{2} + \frac{\pi}{4})$$

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

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

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

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

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

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

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 $k(x)$ and $k(x)$ are expressed by

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

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

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;

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

The wavefunction in the region I

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

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

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: $\psi_n(\xi)$

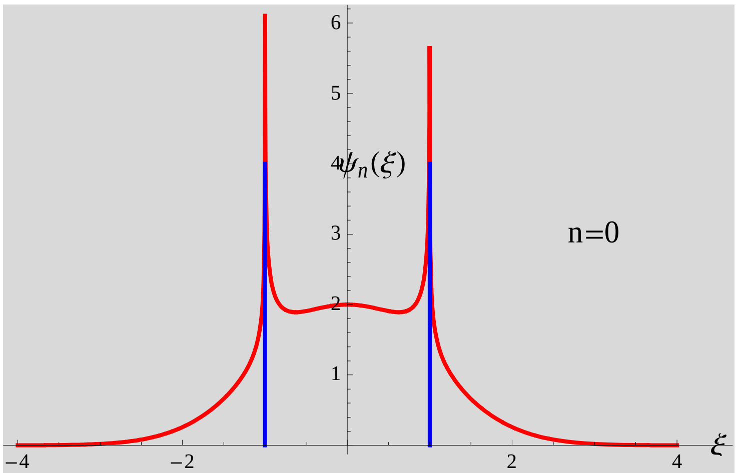
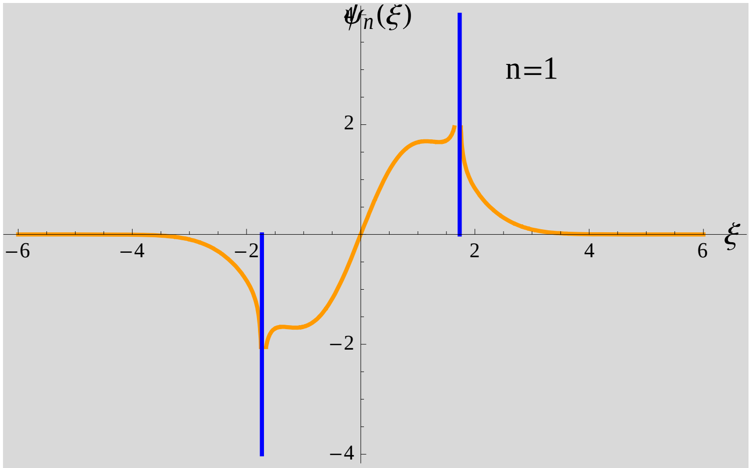
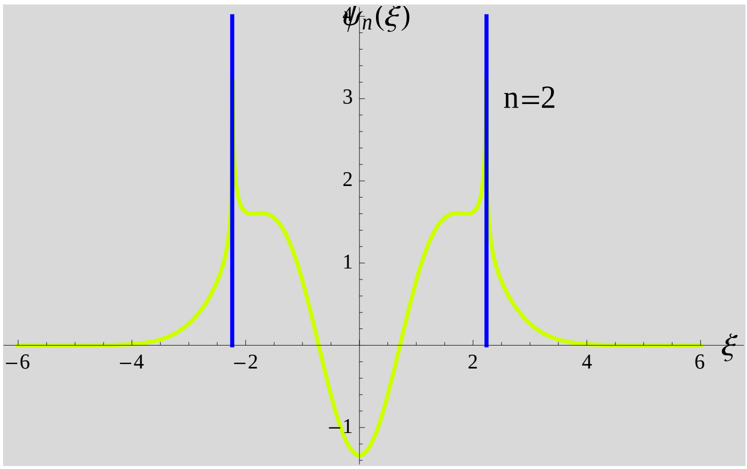


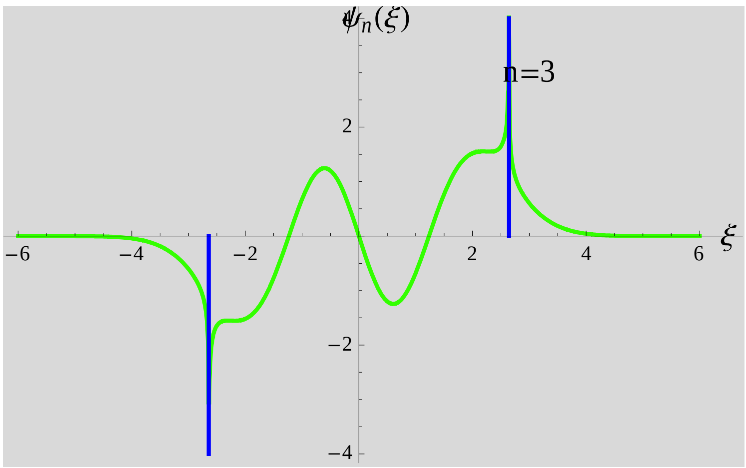
Fig. n = 0 (ground state). The blue lines are classical turning points.



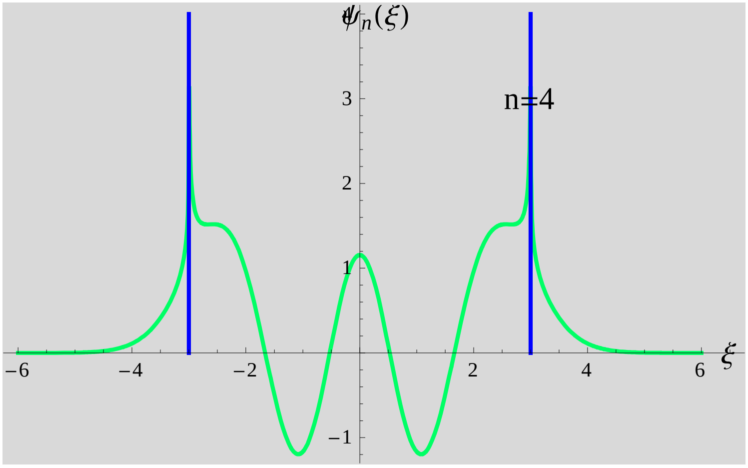
$\psi_n(\xi)$
n=1
2
−2
−4
−6
−4
−2
2
4
6
ξ

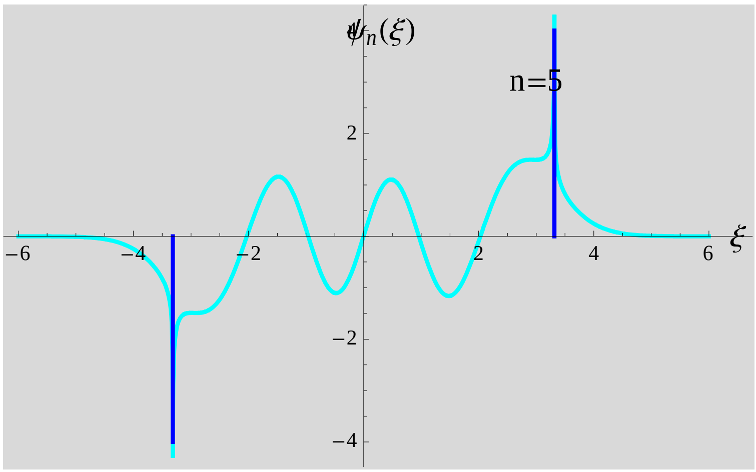


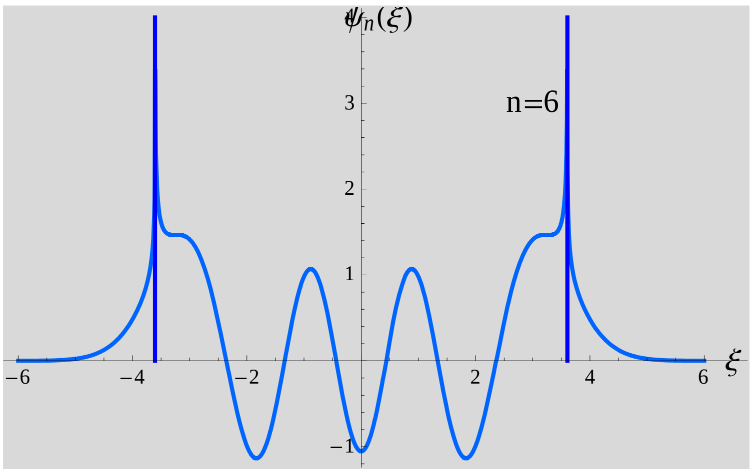
$\psi_n(\xi)$
n=2
3
2
1
−1
−6
−4
−2
2
4
6
ξ



$\psi_n(\xi)$
n=3
2
−2
−4
−6
−4
−2
2
4
6
ξ

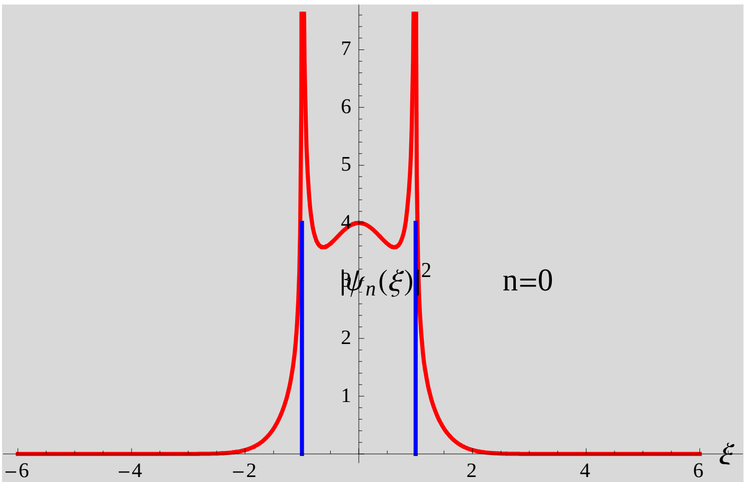


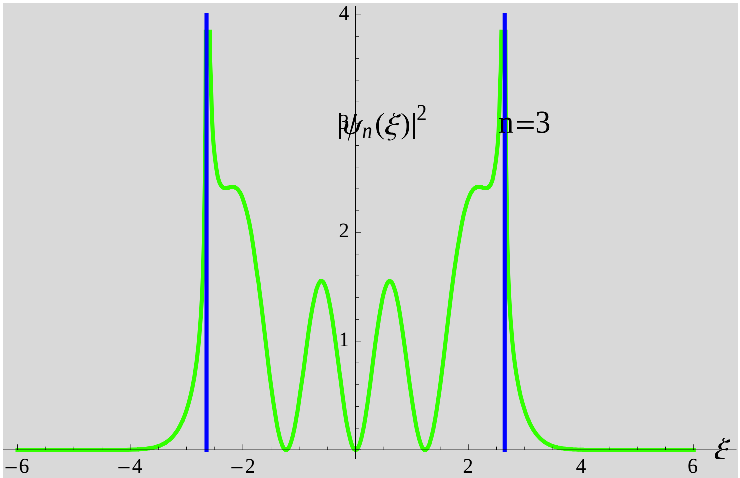


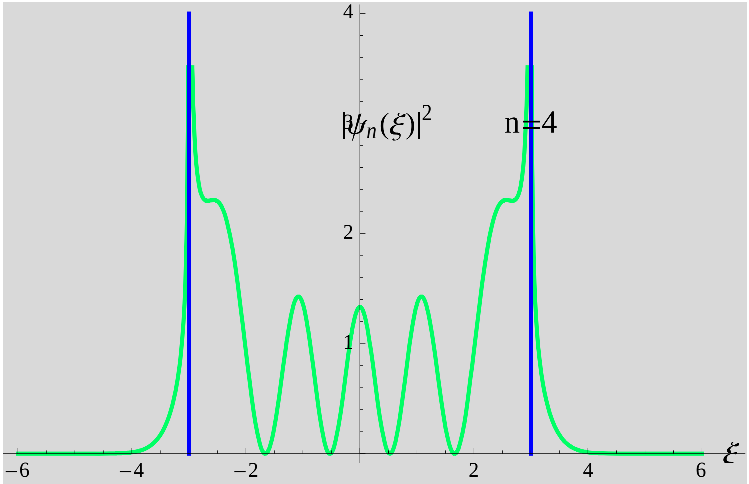


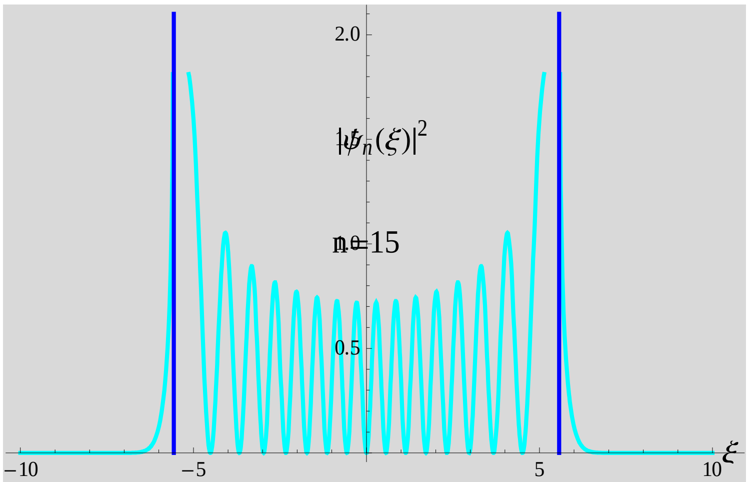
We see that the WKB solution agrees well with the solutions from the quantum mechanics

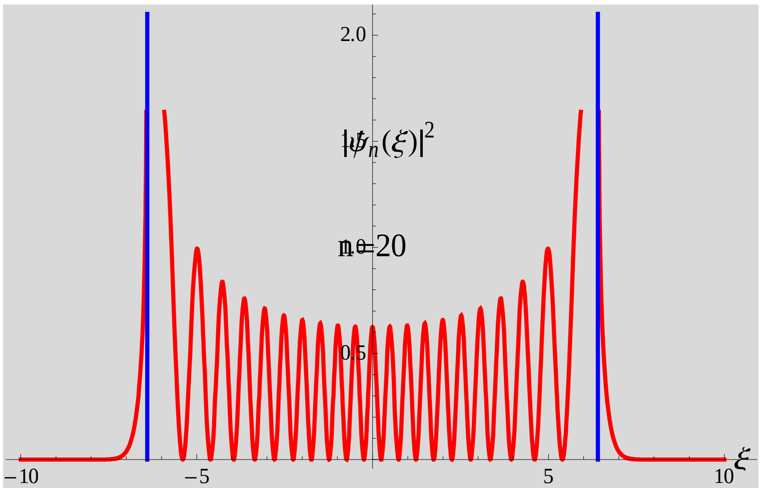
4. Result from Mathematica: $|\psi_n(\xi)|^2$






$|\psi_n(\xi)|^2$
n=4
ξ


$|\psi_n(\xi)|^2$
n=15
ξ


$|\psi_n(\xi)|^2$
n=20
ξ

REFERENCES

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2. David. Bohm, Quantum Theory (Dover Publication, Inc, New York, 1979).
3. Eugen Merzbacher, Quantum Mechanics, 3rd edition (John Wiley & Sons, New York, 1998).
4. Leonard Schiff, Quantum Mechanics (McGraw-Hill Book Company, Inc, New York, 1955).
5. Richard L. Liboff, Introductory Quantum Mechanics, 4th edition (Addison Wesley,

APPENDIX-1: Mathematica program

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

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

```
g11 = 1/4 (2 ξ1 Sqrt[-1 - 2 n1 + ξ1^2] + (1 + 2 n1) (Log[1 + 2 n1] - 2 Log[ξ1 + Sqrt[-1 - 2 n1 + ξ1^2]]));

g21 = 1/4 (π + 2 n1 π + 2 ξ1 Sqrt[1 + 2 n1 - ξ1^2] + (2 + 4 n1) ArcTan[ξ1/Sqrt[1 + 2 n1 - ξ1^2]]);

g31 =
  1/2 (-ξ1 Sqrt[-1 - 2 n1 + ξ1^2] - (1 + 2 n1) Log[-Sqrt[1 + 2 n1]] +
     (1 + 2 n1) Log[ξ1 + Sqrt[-1 - 2 n1 + ξ1^2]]);

ψ1 = 1/Sqrt[Sqrt[ξ1^2 - (2 n1 + 1)]] Exp[-g11] ;

ψ3 = (-1)^n1/Sqrt[Sqrt[ξ1^2 - (2 n1 + 1)]] Exp[-g31] ;

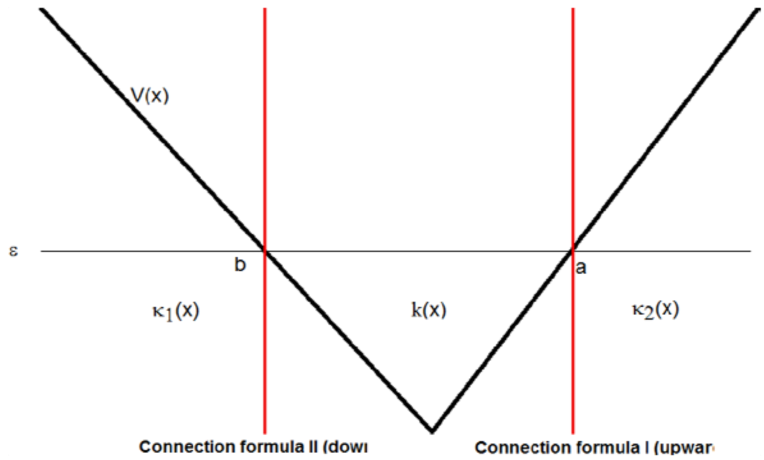
ψ2 = (2 (-1)^n1)/Sqrt[Sqrt[-ξ1^2 + (2 n1 + 1)]] Cos[g21 - π/4] ;

ψ[n_, ξ_] :=
  (ψ3 UnitStep[-ξ1 - Sqrt[2 n1 + 1]] +
      ψ2 (UnitStep[ξ1 + Sqrt[2 n1 + 1]] - UnitStep[ξ1 - Sqrt[2 n1 + 1]]) +
      ψ1 UnitStep[ξ1 - Sqrt[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[{{-Sqrt[2 n1 + 1], 0}, {-Sqrt[2 n1 + 1], (-1)^n1 4}}],
      Line[{{Sqrt[2 n1 + 1], 0}, {Sqrt[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



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

$\Rightarrow$

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

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

$\Rightarrow$

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