One dimensional bound state

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1 One dimensional bound state

As a simple example of the calculation of discrete energy levels of a particle (with mass m) in quantum mechanics, we consider the one dimensional motion of a particle in the presence of a square-well potential barrier (width 2*a* and a depth V_0) as shown below.

$V(x) = 0$ for $|x|>a$, and $-V_0$ for $-a<x<a$.

If the energy of the particle *E* is negative, the particle is confined and in a bound state. Here we discuss the energy eigenvalues and the eigenfunctions for the bound states from the solution of the Schrödinger equation.

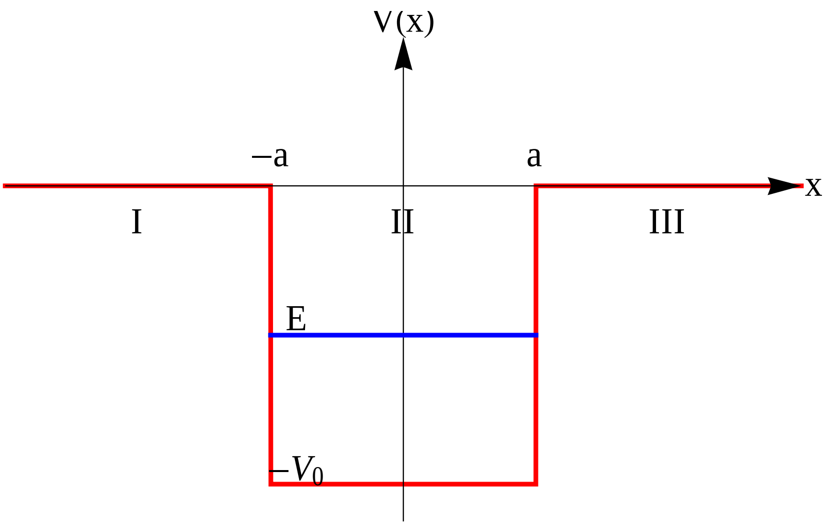

Fig.8 One dimensional square well potential of width 2a and depth V_0.

(a) The parity of the wave function

When potential is an even function (symmetric with respect to *x*), the wave function should have even parity or odd parity.

((**Proof**))

$$[\hat{\pi}, \hat{H}] = 0 .$$

$\hat{\pi}$ is the parity operator.

$$\hat{\pi}^2 = 1 \qquad \hat{\pi}^+ = \hat{\pi} = \hat{\pi}^{-1} .$$

$$\hat{\pi}\hat{x}\hat{\pi} = -\hat{x} . \qquad \hat{\pi}\hat{p}\hat{\pi} = -\hat{p} .$$

$\hat{H}$ is the Hamiltonian.

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}),$$

and

$$\begin{aligned}
\hat{\pi}\hat{H}\hat{\pi} &= \hat{\pi}[\frac{\hat{p}^2}{2m} + V(\hat{x})]\hat{\pi} \\
&= \frac{1}{2m}(\hat{\pi}\hat{p}\hat{\pi})^2 + V(\hat{\pi}\hat{x}\hat{\pi}) \\
&= \frac{1}{2m}(-\hat{p})^2 + V(-\hat{x}) \\
&= \frac{1}{2m}\hat{p}^2 + V(\hat{x})
\end{aligned}.$$

since $V(-\hat{x}) = V(\hat{x})$. Then we have a simultaneous eigenket:

$$\hat{H}|\psi\rangle = E|\psi\rangle, \text{ and } \hat{\pi}|\psi\rangle = \lambda|\psi\rangle.$$

Since $\hat{\pi}^2 = 1$,

$$\hat{\pi}^2|\psi\rangle = \lambda\hat{\pi}|\psi\rangle = \lambda^2|\psi\rangle = |\psi\rangle.$$

Thus we have $\lambda = \pm 1$.

or

$$\hat{\pi}|\psi\rangle = \pm|\psi\rangle,$$

$$\langle x|\hat{\pi}|\psi\rangle = \pm\langle x|\psi\rangle.$$

Since

$$\hat{\pi}|x\rangle = |-x\rangle, \text{ or } \langle x|\hat{\pi}^{+} = \langle x|\hat{\pi} = \langle -x|$$

we have

$$\langle -x|\psi\rangle = \pm\langle x|\psi\rangle,$$

or

$$\psi(-x) = \pm\psi(x) .$$

(b) Wavefunctions

In the Regions I, II, and III, the Schrödinger equation takes the form

$$\frac{d^2}{dx^2}\psi(x) - \kappa^2\psi(x) = 0 \qquad \text{outside the well.}$$

$$\frac{d^2}{dx^2}\psi(x) + k^2\psi(x) = 0 \qquad \text{inside the well.}$$

Here we define

$$\kappa^2 = \frac{2m}{\hbar^2}|E| , \qquad k^2 = \frac{2m}{\hbar^2}(V_0 - |E|) .$$

Here we introduce parameters (β and σ) for convenience,

$$\kappa^2 = \frac{2m}{\hbar^2}|E| = \frac{2mV_0}{\hbar^2}\frac{|E|}{V_0} = \frac{2mV_0a^2}{\hbar^2}\frac{1}{a^2}\frac{|E|}{V_0} = \frac{\beta^2}{a^2}\varepsilon ,$$

or

$$\kappa^2 = \frac{\beta^2}{a^2}\varepsilon ,$$

and

$$k^2 = \frac{2m}{\hbar^2}(V_0 - |E|) = \frac{2mV_0}{\hbar^2}(1 - \frac{|E|}{V_0}) = \frac{1}{a^2}\beta^2(1-\varepsilon) ,$$

where

$$\varepsilon = \frac{|E|}{V_0} , \qquad \text{and} \qquad \beta = \sqrt{\frac{2mV_0a^2}{\hbar^2}} .$$

We note that

$$k^2 + \kappa^2 = \frac{\beta^2}{a^2} ,$$

or

$$\xi^2 + \eta^2 = \beta^2 ,$$

where $ka = \xi$ and $ka = \eta$. The energy ε is given by

$$\varepsilon = \frac{\eta^2}{\beta^2} = 1 - \frac{\xi^2}{\beta^2} .$$

The stationary solution of the three regions are given by

$$\varphi_I(x) = Ae^{\kappa x} ,$$

$$\varphi_{II}(x) = B_1 e^{ikx} + B_2 e^{-ikx} ,$$

$$\varphi_{III}(x) = Ce^{-\kappa x} .$$

(i) The wave function with even parity

$$A = C ,$$
$$B_1 = B_2 \equiv \frac{B}{2} .$$

The wavefunctions can be described by

$$\varphi_I(x) = Ae^{\kappa x} ,$$

$$\varphi_{II}(x) = B\cos(kx) ,$$

$$\varphi_{III}(x) = Ae^{-\kappa x} .$$

The derivatives are obtained by

$$\frac{d\varphi_I(x)}{dx} = A\kappa e^{\kappa x} ,$$

$$\frac{d\varphi_{II}(x)}{dx} = -Bk\sin(kx) ,$$

$$\frac{d\varphi_{III}(x)}{dx} = -A\kappa e^{-\kappa x} .$$

At $x = a$, $\varphi(x)$ and $\dfrac{d\varphi(x)}{dx}$ are continuous. Then we have

$$Ae^{-\kappa a} - B\cos(ka) = 0\,,$$

$$-A\kappa e^{-\kappa a} + Bk\sin(ka) = 0\,,$$

or

$$MX=0,$$

where

$$M = \begin{pmatrix} e^{-\kappa a} & -\cos(ka) \\ -\kappa e^{-\kappa a} & k\sin(ka) \end{pmatrix}, \qquad X = \begin{pmatrix} A \\ B \end{pmatrix}.$$

The condition det$M$=0 leads to

$$k\sin(ka)e^{-\kappa a} = \kappa e^{-\kappa a}\cos(ka)\,,$$

or

$$\tan(ka) = \frac{\kappa}{k} \text{ for the even parity,}$$

or

$$\kappa a = ka\tan(ka) \qquad \text{for the even parity.}$$

or

$$\eta = \xi\tan\xi\,.$$

The constants A, B, and C are given by

$$A = C = Be^{\kappa a}\cos(ka)\,.$$

The condition of the normalization leads to the value of B.

(ii) The wave function with odd parity

$$A = -C\,,$$

$$B_1 = -B_2 \equiv \frac{B}{2i}.$$

The wavefunctions are given by

$$\varphi_I(x) = -Ae^{\kappa x},$$

$$\varphi_{II}(x) = B\sin(kx),$$

$$\varphi_{III}(x) = Ae^{-\kappa x}.$$

The derivatives are obtained as

$$\frac{d\varphi_I(x)}{dx} = -A\kappa e^{\kappa x},$$

$$\frac{d\varphi_{II}(x)}{dx} = Bk\cos(kx),$$

$$\frac{d\varphi_{III}(x)}{dx} = -A\kappa e^{-\kappa x}.$$

At $x = a$, $\varphi(x)$ and $\frac{d\varphi(x)}{dx}$ are continuous. Then we have

$$-Ae^{-\kappa a} + B\sin(ka) = 0,$$

$$-A\kappa e^{-\kappa a} - Bk\cos(ka) = 0,$$

or

$$MX=0,$$

where

$$M = \begin{pmatrix} -e^{-\kappa a} & \sin(ka) \\ -\kappa e^{-\kappa a} & -k\cos(\frac{ka}{2}) \end{pmatrix}, \qquad X = \begin{pmatrix} A \\ B \end{pmatrix}.$$

The condition det$M$=0 leads to

$$k\cos(ka)e^{-\kappa a} = -\kappa e^{-\kappa a}\sin(ka),$$

or

$$\kappa a = -ka\cot(ka) \qquad \text{for the odd parity,}$$

or

$$\eta = -\xi\cot\xi .$$

We solve this eigenvalue problem using the Mathematica. The result is as follows.

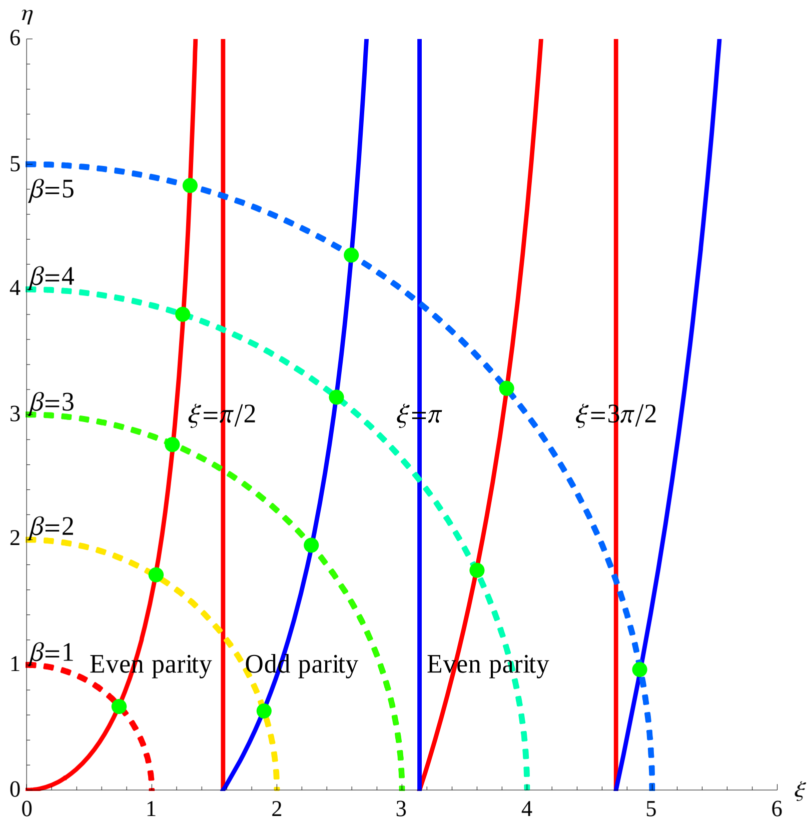

Fig.9 Graphical solution. One solution with even parity for 0<*β*<*π*/2. One solution with even parity and one solution with odd parity for *π*/2<*β*<*π*. Two solutions with even parity and one solution with odd parity for *π*<*β*<3*π*/2. Two solutions with even parity and two solutions with odd parity for 3*π*/2<*β*<2*π*. $\eta = \xi\tan\xi$ for the even parity (red lines). $\eta = -\xi\cot\xi$ for the odd parity (blue lines). The circles are denoted by $\xi^2 + \eta^2 = \beta^2$. The parameter β is changed as β = 1, 2, 3, 4, and 5. $\varepsilon = \frac{|E|}{V_0} = \frac{\eta^2}{\beta^2} = 1 - \frac{\xi^2}{\beta^2}$. $\xi = ka$ and $\eta = \kappa a$.

The normalized wavefunction for the even parity and odd parity are given by

$$\psi eI = \frac{e^{\eta + x\eta}\,\text{Cos}[\xi]}{\sqrt{1 + \frac{\text{Cos}[\xi]^2}{\eta} + \frac{\text{Sin}[2\xi]}{2\xi}}};\quad \psi eII = \frac{\text{Cos}[x\,\xi]}{\sqrt{1 + \frac{\text{Cos}[\xi]^2}{\eta} + \frac{\text{Sin}[2\xi]}{2\xi}}};$$

$$\psi eIII = \frac{e^{\eta - x\eta}\,\text{Cos}[\xi]}{\sqrt{1 + \frac{\text{Cos}[\xi]^2}{\eta} + \frac{\text{Sin}[2\xi]}{2\xi}}};$$

$$\psi oI = -\frac{e^{\eta + x\eta}\,\text{Sin}[\xi]}{\sqrt{1 + \frac{\text{Sin}[\xi]^2}{\eta} - \frac{\text{Sin}[2\xi]}{2\xi}}};\quad \psi oII = \frac{\text{Sin}[x\,\xi]}{\sqrt{1 + \frac{\text{Sin}[\xi]^2}{\eta} - \frac{\text{Sin}[2\xi]}{2\xi}}};$$

$$\psi oIII = \frac{e^{\eta - x\eta}\,\text{Sin}[\xi]}{\sqrt{1 + \frac{\text{Sin}[\xi]^2}{\eta} - \frac{\text{Sin}[2\xi]}{2\xi}}};$$

for the regions I, II, and III, where ψ_e is the wavefunction with the even parity and ψ_o is the wavefunction with the odd parity.

$\beta = 1$

$\xi_{11} = 0.739085$	$\eta_{11} = 0.673612$	$\varepsilon_{11} = 0.453753$	even

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$\beta = 2$

$\xi_{21} = 1.02987$	$\eta_{21} = 1.71446$	$\varepsilon_{21} = 0.734844$	even
$\xi_{22} = 1.89549$	$\eta_{22} = 0.638045$	$\varepsilon_{22} = 0.101775$	odd

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$\beta = 3$

$\xi_{31} = 1.17012$	$\eta_{31} = 2.76239$	$\varepsilon_{31} = 0.847869$	even
$\xi_{32} = 2.27886$	$\eta_{32} = 1.9511$	$\varepsilon_{32} = 0.422976$	odd

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$\beta = 4$

$\xi_{41} = 1.25235$	$\eta_{41} = 3.7989$	$\varepsilon_{41} = 0.901976$	even
$\xi_{42} = 2.47458$	$\eta_{42} = 3.14269$	$\varepsilon_{42} = 0.617279$	odd
$\xi_{43} = 3.5953$	$\eta_{43} = 1.75322$	$\varepsilon_{43} = 0.192111$	even

$\beta = 5$

ξ_{51} = 1.30644	η_{51} = 4.8263,	ε_{51} = 0.931729	even
ξ_{52} = 2.59574	η_{52} = 4.27342,	ε_{52} = 0.730486	odd
ξ_{53} = 3.83747	η_{53} = 3.20528,	ε_{53} = 0.410954	even
ξ_{54} = = 4.9063	η_{54} =.963467,	ε_{54} = 0.0371307	odd

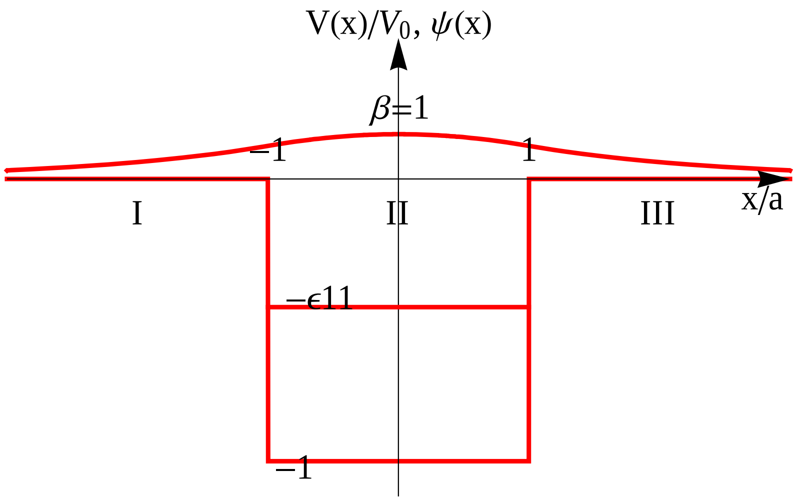

Fig.10 Square well potential $V(x)$ of width $2a$ and depth V_0. β = 1 and the corresponding wavefunction $\psi(x)$ which is normalized. There is one bound state (even parity) (- ε_{11} = -0.45735), where $\varepsilon = |E|/V_0$.

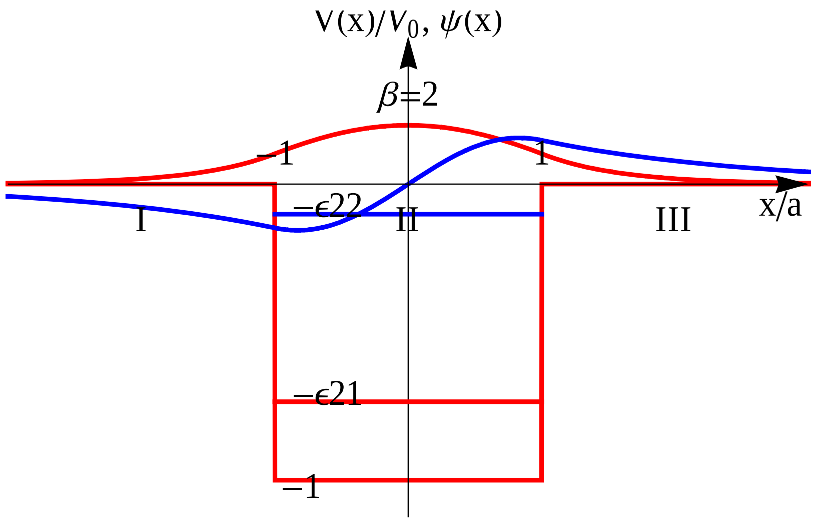

Fig.11 β = 2. There are two bound states. (i) The bound state (denoted by red) with even parity (- ε_{21} = -0.734844). (ii) The bound state (denoted by blue) with odd parity (-ε_{22} = -0.101775).

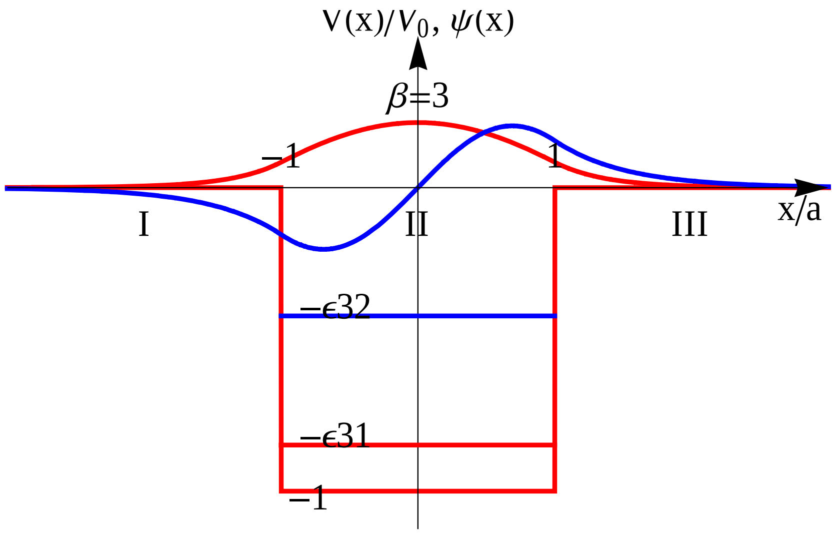

Fig.12 β = 3. There are two bound states. (i) The bound state (denoted by red) with even parity (-ε_{31} = -0.847869). (ii) The bound state (denoted by blue) with odd parity (-ε_{32} = -0.422976).

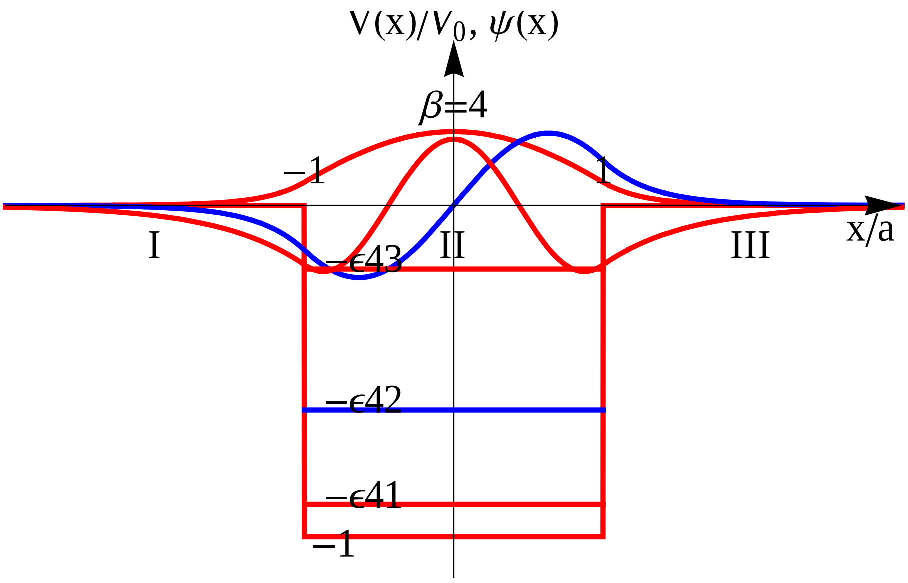

Fig.13 β = 4. There are three bound states. (i) The bound state (denoted by red) with even parity (-ε_{41} = -0.901976). (ii) The bound state (denoted by blue) with odd parity ($-\varepsilon_{42}$ = -0.617279). (iii) The bound state (denoted by red) with even parity ($-\varepsilon_{43}$ = -0.192111).

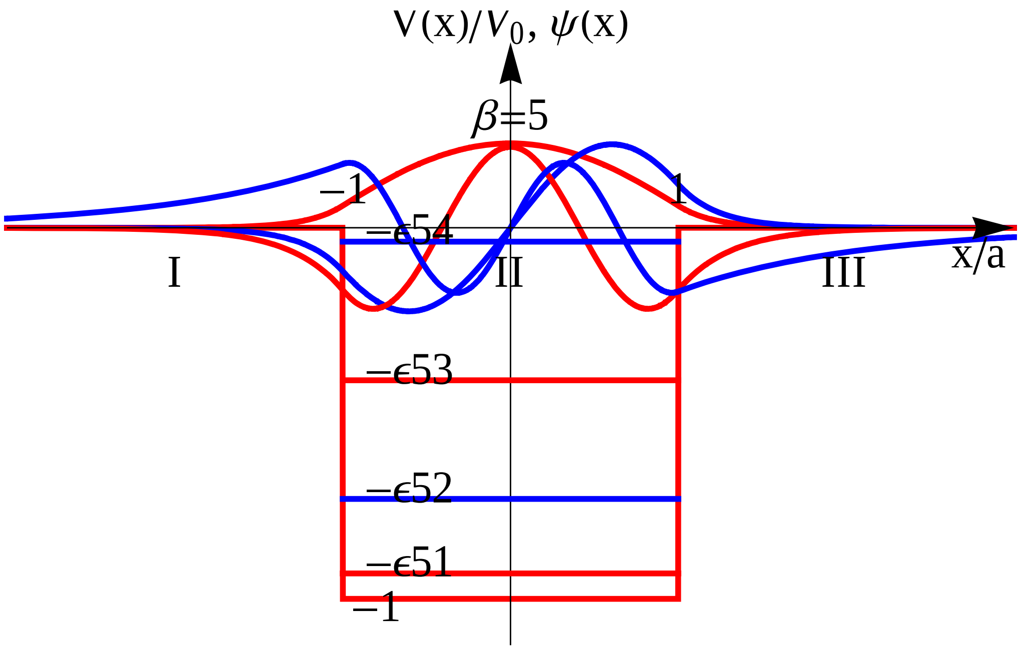

Fig.14 β = 5. There are four bound states. (i) The bound state (denoted by red) with even parity ($-\varepsilon_{51}$ = -0.931729). (ii) The bound state (denoted by blue) with odd parity ($-\varepsilon_{52}$ = -0.730486). (iii) The bound state (denoted by red) with even parity ($-\varepsilon_{53}$ = -0.410954). (iv) The bound state (denoted by blue) with odd parity ($-\varepsilon_{54}$ = -0.0371307).

REFERENCES

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2. E. Merzbacher, Quantum Mechanics Third edition (John Wiley and Sons, New York, 1998,