Chapter 6
Sturm Liouville Theory

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Jacques Charles François Sturm (September 29, 1803 – December 15, 1855) was a French mathematician of German heritage.

http://en.wikipedia.org/wiki/Jacques_Charles_Fran%C3%A7ois_Sturm

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Joseph Liouville (24 March 1809 – 8 September 1882) was a French mathematician.

http://en.wikipedia.org/wiki/Joseph_Liouville

6.1 Self-adjoint differential equation

$$Ly = p_0(x)y'' + p_1(x)y' + p_2(x)y .$$

(i) $p_0(x)$, $p_1(x)$, and $p_2(x)$ are real functions of x.
(ii) $p_0(x)$, $p_0'(x)$, $p_0''(x)$, $p_1(x)$, $p_1'(x)$, and $p_2(x)$ are continuous

((**Dirac notation**))

$$\langle v|\hat{L}|u\rangle = \int_a^b v^* L u dx = \int_a^b v^*[p_0 u'' + p_1 u' + p_2 u]dx .$$

$$\begin{aligned}\int_a^b v^* p_0 u'' dx &= [v^* p_0 u']_a^b - \int_a^b (v^* p_0)' u' dx \\ &= [v^* p_0 u']_a^b - [(v^* p_0)' u]_a^b + \int_a^b (p_0 v^*)'' u dx\end{aligned}.$$

$$\int_a^b v^* p_1 u' dx = [v^* p_1 u]_a^b - \int_a^b (v^* p_1)' u dx .$$

Then

$$\langle v|\hat{L}|u\rangle = \int_a^b [(p_0 v^*)'' - (p_1 v^*)' + p_2 v^*] u dx + [v^* p_0 u' - (v^* p_0)' u + v^* p_1 u]_a^b .$$

Here note that

$$\begin{aligned}[v^* p_0 u' - (v^* p_0)' u + v^* p_1 u]_a^b &= [v^* p_0 u' - (v^{*\prime} p_0 + v^* p_0')u + v^* p_1 u]_a^b \\ &= [(u' v^* - u v^{*\prime}) p_0 + (p_1 - p_0') u v^*]_a^b\end{aligned}.$$

Then we have

$$\langle v|\hat{L}|u\rangle = \int_a^b [(p_0 v^*)'' - (p_1 v^*)' + p_2 v^*] u dx + [(u' v^* - u v^{*\prime}) p_0 + (p_1 - p_0') u v^*]_a^b .$$

The terms at the boundary ($x = a$ and $x = b$) also vanish. So we get

$$\langle v|\hat{L}|u\rangle = \int_a^b [(p_0 v^*)'' - (p_1 v^*)' + p_2 v^*] u dx = \int_a^b u \overline{L} v^* dx ,$$

or

$$\langle v|\hat{L}|u\rangle^* = \int_a^b [(p_0 v)''-(p_1 v)'+p_2 v]u^* dx = \int_a^b u^* \overline{L} v dx ,$$

where the adjoint operator $\overline{L}$ is defined as

$$\overline{L}y = (p_0 y)''-(p_1 y)'+p_2 y .$$

Thus we have

$$\langle u|\hat{L}^{+}|v\rangle = \langle v|\hat{L}|u\rangle^* = \int_a^b u^* \overline{L} v dx . \qquad (1)$$

(here we define the Hermitian conjugate operator).

Note that

$$\langle u|\hat{L}|v\rangle = \int_a^b u^* L v dx , \qquad (2)$$

from the definition. Suppose that $\overline{L}v = Lv$. Then we have

$$\langle u|\hat{L}^{+}|v\rangle = \langle u|\hat{L}|v\rangle . \qquad \text{(Hermitian)}.$$

When $\overline{L}y = Ly$,

$$\overline{L}y = (p_0 y)''-(p_1 y)'+p_2 y = p_0 y''+p_1 y'+p_2 y ,$$

or

$$p_0 y''+2p_0' y'+p_0'' y-(p_1' y+p_1 y') = p_0 y''+p_1 y' ,$$

or

$$2(p_0'-p_1)y'+(p_0''-p_1')y = 0 .$$

When the condition $p_0' = p_1$ is satisfied,

$$Ly = \overline{L}y = \frac{d}{dx}[p_0(x)y'] + p_2(x)y .$$

The operator L is said to be Hermitian with respect to the functions u and v, satisfying the boundary conditions.

((**Mathematica**))

(a) Example-1

L1: a linear operator
L1B: an adjoint operator

What is the condition for the self-adjoint?

```
Clear["Global`*"];

L1 := p0[x] D[#, {x, 2}] + p1[x] D[#, x] + p2[x] # &

L1B := D[p0[x] #, {x, 2}] - D[p1[x] #, x] + p2[x] # &

eq1 = L1[ψ[x]] // Simplify

p2[x] ψ[x] + p1[x] ψ′[x] + p0[x] ψ″[x]

eq2 = L1B[ψ[x]] // Simplify

p2[x] ψ[x] - p1[x] ψ′[x] + 2 p0′[x] ψ′[x] +
 ψ[x] (-p1′[x] + p0″[x]) + p0[x] ψ″[x]

eq12 = Collect[(eq1 - eq2), {ψ'[x], ψ[x]}]

(2 p1[x] - 2 p0′[x]) ψ′[x] + ψ[x] (p1′[x] - p0″[x])
```

(b) Example-2

Arfken 10 - 1 - 8

For a second-order differential operator L that is self-adjoint, show that
y2 L(y1)-y1 L(y2)=[p(y1'y2-y1y2')]'

```
Clear["Global`*"]

LS := D[p[x] D[#, x], x] + q[x] # &

eq1 = y2[x] LS[y1[x]] - y1[x] LS[y2[x]] // Simplify

y2[x] (p′[x] y1′[x] + p[x] y1″[x]) - y1[x] (p′[x] y2′[x] + p[x] y2″[x])

eq11 = Collect[eq1, {p[x], p'[x]}]

p′[x] (y2[x] y1′[x] - y1[x] y2′[x]) + p[x] (y2[x] y1″[x] - y1[x] y2″[x])

eq2 = D[p[x] (y2[x] y1′[x] - y1[x] y2′[x]), x]

p′[x] (y2[x] y1′[x] - y1[x] y2′[x]) + p[x] (y2[x] y1″[x] - y1[x] y2″[x])

eq11 - eq2

0
```

(c) Example-3

Arfken 10 - 1 - 7
Given that Lu = 0 and gLu is self adjoint, show that for the adjoint operator $\overline{L}$, $\overline{L}(gu) = 0$.

We define the adjoint operator as follows.

```
L1 := p0[x] D[#, {x, 2}] + p1[x] D[#, x] + p2[x] # &

L1B := D[p0[x] #, {x, 2}] - D[p1[x]  #, x] + p2[x] # &

eq1 = L1[u[x]]
```

p2[x] u[x] + p1[x] u′[x] + p0[x] u″[x]

```
eq11 = Solve[eq1 == 0, u''[x]]
```

$$\left\{\left\{u''[x] \to \frac{-p2[x]\, u[x] - p1[x]\, u'[x]}{p0[x]}\right\}\right\}$$

```
eq2 = g[x] L1[u[x]] // Expand
```

g[x] p2[x] u[x] + g[x] p1[x] u′[x] + g[x] p0[x] u″[x]

The condition that gLu is self - adjoint:

```
eq31 = Coefficient[g[x] L1[u[x]], u''[x]]
```

g[x] p0[x]

```
eq32 = Coefficient[g[x] L1[u[x]], u'[x]]
```

g[x] p1[x]

```
eq33 = D[eq31, x] - eq32
```

-g[x] p1[x] + p0[x] g′[x] + g[x] p0′[x]

```
eq34 = D[eq33, x]
```

-p1[x] g′[x] + 2 g′[x] p0′[x] - g[x] p1′[x] + p0[x] g″[x] + g[x] p0″[x]

We now show that L1B[g u] = 0

```
eq4 = L1B[g[x] u[x]] // Simplify
```

```
-p1[x] u[x] g′[x] + 2 u[x] g′[x] p0′[x] + 2 p0[x] g′[x] u′[x] +
 p0[x] u[x] g″[x] + g[x] (p2[x] u[x] - p1[x] u′[x] +
    2 p0′[x] u′[x] + u[x] (-p1′[x] + p0″[x]) + p0[x] u″[x])
```

```
eq41 = Collect[eq4 /. eq11[[1]], {u′[x], u[x]}] // Simplify
```

```
2 (p0[x] g′[x] + g[x] (-p1[x] + p0′[x])) u′[x] +
 u[x] (-p1[x] g′[x] + 2 g′[x] p0′[x] + p0[x] g″[x] + g[x] (-p1′[x] + p0″[x]))
```

```
eq42 = Coefficient[eq41, u'[x]]
```

```
2 (p0[x] g′[x] + g[x] (-p1[x] + p0′[x]))
```

```
eq43 = Coefficient[eq41, u[x]]
```

```
-p1[x] g′[x] + 2 g′[x] p0′[x] + p0[x] g″[x] + g[x] (-p1′[x] + p0″[x])
```

From eq33 and eq34, we find that

```
eq51 = eq42 - 2 eq33 // Simplify
```

```
0
```

```
eq52 = eq43 - eq34 // Simplify
```

```
0
```

6.2 Formation of self adjoint differential equation

Any linear 2nd differential equation can be put in this form by multiplying by an appropriate function *f*(*x*).

Suppose that

$$Ly = p_0 y'' + p_1 y' + p_2 y \text{ (general case).} \tag{1}$$

Multiplying this Eq.(1) by *f*

$$f(Ly) = fp_0 y'' + fp_1 y' + fp_2 y = \frac{d}{dx}[fp_0 y'] + fp_2 y,$$

or

$$\frac{d}{dx}(fp_0) = fp_1,$$

or

$$\frac{d(fp_0)}{fp_0} = \frac{p_1}{p_0}dx,$$

or

$$f(x) = \frac{1}{p_0(x)}\exp(\int^x \frac{p_1(t)}{p_0(t)}dt).$$

For a self-adjoint *L* we have

$$Ly = \frac{d}{dx}[p(x)y'] + q(x)y.$$

6.3 Eigenvalue problem I

We now examine the differential equation

$$Ly + \lambda w(x)y = 0.$$

λ is called the eigenvalue and $y(x)$ is called the eigenfunction for a particular λ. $w(x)$ is the weight function.

Boundary condition:

(i)

$$Ay(a) + By'(a) = 0$$
$$Cy(b) + Dy'(b) = 0,$$

where *A*. *B*, *C*, and *D* are given constants.

(ii) Periodic boundary condition

$$y(x) = y(x + b - a).$$

6.4 Example

(A) Legendre differential equation

$$(1 - x^2)y'' - 2xy' + n(n+1)y = 0,$$

$$p_0(x) = 1 - x^2, \qquad p_1(x) = -2x = p_0'(x),$$

Thus this is self-adjoint

$$Ly + \lambda wy = 0,$$

with

$$Ly = \frac{d}{dx}[(1-x^2)y'],$$

$$\begin{aligned} w &= 1 \\ \lambda &= n(n+1) \end{aligned}.$$

(B) Laguerre's differential equation

$$xy'' + (1-x)y' + ay = 0,$$

with

$p_0(x) = x$, $\qquad p_1(x) = 1-x$,

Since $p_0'(x) = 1 \neq p_1(x)$, this is not a self-adjoint. We multiply this Eq. by a function *f*,

$$\begin{aligned} f &= \frac{1}{p_0(x)}\exp\left(\int^x \frac{p_1(t)}{p_0(t)}dt\right) \\ &= \frac{1}{x}\exp\left(\int^x \frac{1-t}{t}dt\right) \\ &= \frac{1}{x}\exp(\ln x - x) = \frac{1}{x}e^{-x}x = e^{-x} \end{aligned}.$$

Then we have

$$xe^{-x}y'' + (1-x)e^{-x}y' + ae^{-x}y = 0,$$

or

$$Ly + \lambda wy = 0,$$

with

$$\begin{aligned} Ly &= \frac{d}{dx}(xe^{-x}y') \\ \lambda &= a \\ w &= e^{-x} \end{aligned}.$$

(C) Hermite differential equation

$$y''-2xy'+2\alpha y=0,$$

$$p_0(x)=1, \qquad p_1(x)=-2x,$$

Since $p_0'(x)=0\neq p_1(x)=-2$, this is not a self-adjoint. We multiply this Eq. by a function *f*,

$$f=\frac{1}{p_0(x)}\exp\left(\int^x\frac{p_1(t)}{p_0(t)}dt\right)=\exp\left[\int^x(-2t)dt\right]=e^{-x^2}.$$

Then we have

$$e^{-x^2}y''-2xe^{-x^2}y'+2\alpha e^{-x^2}y=0,$$

or

$$Ly+\lambda wy=0,$$

with

$$Ly=\frac{d}{dx}(e^{-x^2}y')$$
$$\lambda=2\alpha \qquad .$$
$$w=e^{-x^2}$$

(D) Bessel differential equation

$$x^2y''+xy'+(x^2-n^2)y=0,$$

$$p_0(x)=x^2, \qquad p_1(x)=x.$$

Since $p_0'(x)=2x\neq p_1(x)=x$, this is not a self-adjoint. We multiply this Eq. by a function *f*,

$$f=\frac{1}{p_0(x)}\exp\left(\int^x\frac{p_1(t)}{p_0(t)}dt\right)=\frac{1}{x^2}\exp\left[\int^x\frac{t}{t^2}dt\right]=\frac{1}{x^2}\exp(\ln x)=\frac{1}{x}.$$

Then we have

$$xy''+y'+(x-\frac{n^2}{x})y=0,$$

or

$$Ly+\lambda wy=0,$$

with

$$Ly=\frac{d}{dx}(xy')-\frac{n^2}{x}y$$
$$\lambda=1 \quad .$$
$$w=x$$

6.5. Eigenvalue problem II

L is a self-adjoint differential operator. *u* and *v* are the solutions of

$$Ly+\lambda wy=0$$

which satisfies the boundary condition

$$[v^*(pu')]_a^b=0 \text{ and } [u^*(pv')]_a^b=0$$

We now examine

$$\begin{aligned}\langle v|\hat{L}|u\rangle &= \int_a^b v^* Lu dx = \int_a^b v^*[(pu')'+qu]dx \\ &= [v^*(pu')]_a^b - \int_a^b v^{*}{}' pu' dx + \int_a^b v^* qu dx \\ &= -\int_a^b v^{*}{}' pu' dx + \int_a^b v^* qu dx = -[v^*(pu')]_a^b + \int_a^b (pv^{*}{}')' u dx + \int_a^b v^* qu dx \\ &= \int_a^b (pv^{*}{}')' u dx + \int_a^b v^* qu dx = \int_a^b u L v^* u dx = \langle u|\hat{L}|v\rangle^* = \langle v|\hat{L}^+|u\rangle\end{aligned}$$

Then we have $\hat{L}^+ = \hat{L}$.

The Hermite operators have three properties that are of extreme importance in physics.

A. The eigenvalues are real.
B. The eigenfunctions are orthogonal.
C. The eigenfunctions form a complete set.

A. Real eigenvalue

Let

$$Lu_j + \lambda_j w u_j = 0,$$

$$Lu_i + \lambda_i w u_i = 0$$

Then taking the complex conjugate

$$Lu_j^* + \lambda_j^* w u_j^* = 0$$

Here L is a real operator (p and q are real functions of x) and $w(x)$ is a real function. But we permit λ_i and λ_j to be complex.

$$(u_j^* L u_i - u_i L u_j^*) = (\lambda_j^* - \lambda_i) w u_i u_j^*,$$

$$\int_a^b u_j^* L u_i dx - \int_a^b u_i L u_j^* dx = (\lambda_j^* - \lambda_i) \int_a^b w u_i u_j^* dx.$$

Since L is Hermitian, the left-hand side vanishes,

$$\int_a^b u_j^* L u_i dx - \int_a^b u_i L u_j^* dx = \langle u_j | \hat{L} | u_i \rangle - \langle u_i | \hat{L} | u_j \rangle^* = \langle u_j | \hat{L} | u_i \rangle - \langle u_j | \hat{L}^+ | u_i \rangle = 0,$$

$$(\lambda_j^* - \lambda_i) \int_a^b w u_i u_j^* dx = 0.$$

If $i = j$,

$$(\lambda_i^* - \lambda_i) \int_a^b w |u_i|^2 dx = 0.$$

Since $\int_a^b w |u_i|^2 dx = 1$ (normalization), we have

$$\lambda_i^* - \lambda_i = 0.$$

B. Orthogonal eigenfunctions

If we take $i \neq j$ and $\lambda_i \neq \lambda_j$, the integral of the product of the two different eigenfunctions vanish.

$$\int_a^b w u_i u_j^* dx = 0 .$$

We say that the eigenfunctions $u_i(x)$ and $u_j(x)$ are orthogonal with respect to the weighting function $w(x)$ over the interval $[a,b]$. We should mention that one does in the case of $\lambda_i = \lambda_j$ ($i \neq j$) – when one has a degeneracy – so the functions $u_i(x)$ and $u_j(x)$ are linearly independent but not orthogonal.

C. Completeness

For any function $\psi(x)$, $\psi(x)$ can be expressed by

$$\psi(x) = \sum_n a_n u_n(x) .$$

The expansion coefficient is determined by the orthogonality of the u_n's.

$$a_n = \int_a^b u_n^*(x) w(x) \psi(x) dx ,$$

where

$$\int_a^b u_n^*(x) w(x) u_m(x) dx = \delta_{n.m} .$$

6.6 Simple differential operator: a particle in a box

We consider a simple case where

$$L = \frac{d^2}{dx^2} \qquad \text{and} \qquad w(x) = 1 .$$

This operator is Hermitian since $p(x) = 1$ and $q(x) = 0$. The eigenfunctions and eigenvalues of this operator satisfy the equation,

$$L u_n + \lambda_n u_n = 0$$

or

$$\frac{d^2}{dx^2} u_n + \lambda_n u_n = 0 .$$

where $\lambda_n = -k_n{}^2$. The solution of this differential equation is

$$u_n(x) = A_n \cos(k_n x) + B_n \sin(k_n x)$$

If we specify the boundary conditions that $u_n(x=0) = u_n(x=a) = 0$, then we have

$$A_n = 0. \qquad \text{and} \qquad k_n = \frac{\pi}{a} n \qquad (n = 1, 2, 3, ...).$$

Then we have the normalized eigenfunction

$$u_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{\pi n}{a} x),$$

with the eigenvalue

$$\lambda_n = -\left(\frac{\pi n}{a}\right)^2.$$

This problem is the same as for the one dimensional Schrodinger equation of a particle in a well potential,

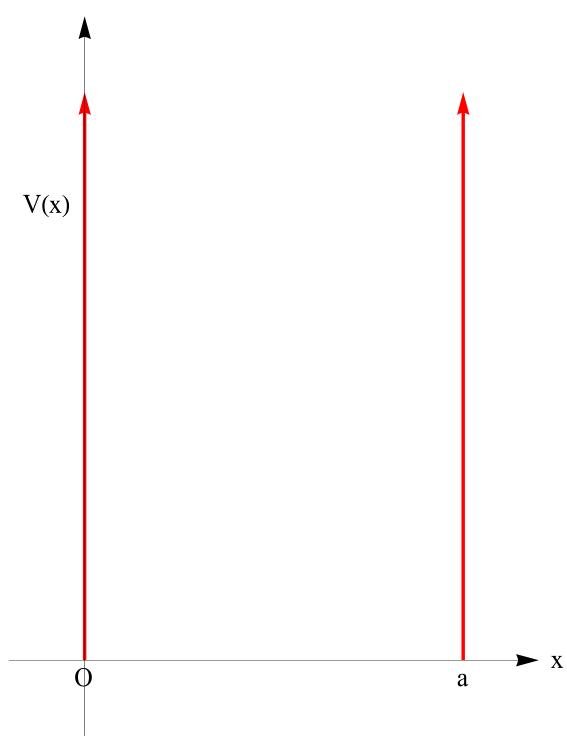


Fig.1 The infinite square-well potential energy.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E_n\psi_n(x)$$

or

$$\frac{d^2}{dx^2}\psi_n(x) + k_n{}^2\psi_n(x) = 0$$

where the energy eigenvalue is

$$E_n = \frac{\hbar^2}{2m}k_n{}^2.$$

Under the boundary condition that $\psi_n(x=0) = \psi_n(x=a) = 0$, then we have

$$k_n = \frac{\pi}{a}n \qquad (n = 1, 2, 3,.....).$$

and the normalized wave function

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin(\frac{\pi n x}{a})$$

with

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2.$$

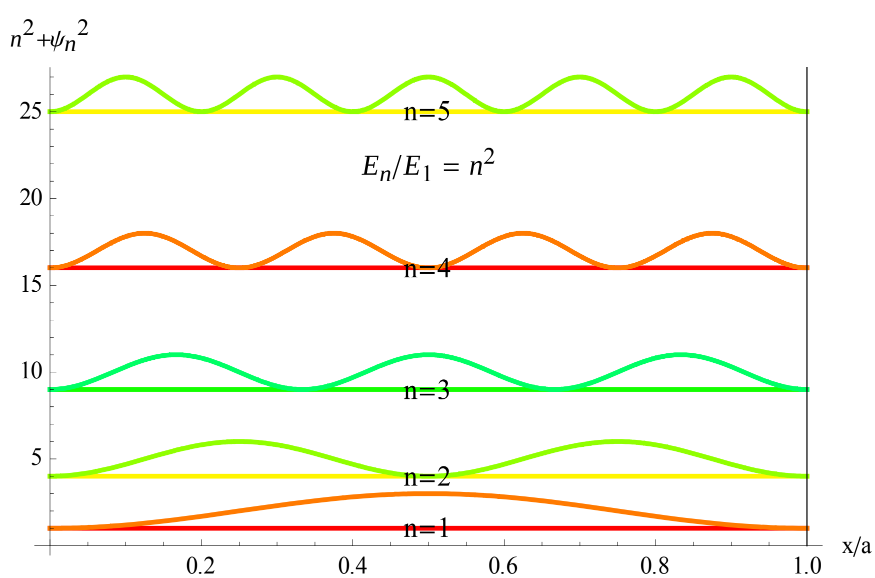


Fig.2 The energy level E_n is given by $E_n = E_1 n^2$. $E_1 = \dfrac{\hbar^2\pi^2}{2ma^2}$. Plot of $(n^2 + \psi_n{}^2)$ as a function of x/a.

6.7 One dimensional harmonic oscillator: Quantum Mechanics

The commutation relation;

$$[\hat{x}, \hat{p}] = i\hbar .$$

The Hamiltonian of the simple harmonics

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{x}^2 .$$

The eigenvalue problem of the simple harmonics in quantum mechanics is given by

$$\hat{H}|n\rangle = \varepsilon_n |n\rangle ,$$

with

$$\varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_0 ,$$

where n = 0, 1, 2, 3,....

Here we introduce the creation operator and annihilation operators given by

$$\hat{a} = \frac{\beta}{\sqrt{2}}\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\hat{x} + \frac{i\hat{p}}{\sqrt{m\hbar\omega_0}}\right),$$

$$\hat{a}^+ = \frac{\beta}{\sqrt{2}}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega_0}{\hbar}}\hat{x} - \frac{i\hat{p}}{\sqrt{m\hbar\omega_0}}\right),$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}} , \qquad \text{(the unit of } \beta \text{ is cm}^{-1}\text{).}$$

The operators $\hat{x}$ and $\hat{p}$ are expressed in terms of $\hat{a}$ and $\hat{a}^+$,

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\left(\hat{a} + \hat{a}^{+}\right) = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a} + \hat{a}^{+}\right),$$

$$\hat{p} = \frac{1}{\sqrt{2}\beta}\frac{m\omega_0}{i}\left(\hat{a} - \hat{a}^{+}\right) = \frac{1}{i}\sqrt{\frac{m\hbar\omega_0}{2}}\left(\hat{a} - \hat{a}^{+}\right).$$

Note that

$$[\hat{x}, \hat{p}] = \frac{1}{\left(\sqrt{2}\beta\right)^2}\frac{m\omega_0}{i}\left[\hat{a} + \hat{a}^{+}, \hat{a} - \hat{a}^{+}\right] = -\frac{\hbar}{i}\left[\hat{a}, \hat{a}^{+}\right],$$

then we have

$$\left[\hat{a}, \hat{a}^{+}\right] = \hat{1}.$$

Since

$$\hat{a}^{+}\hat{a} = \frac{\beta^2}{2}\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)\left(\hat{x} + \frac{i\hat{p}}{m\omega_0}\right) = \frac{\beta^2}{2}\left(\hat{x}^2 + \frac{\hat{p}^2}{m^2\omega_0^2} - i\frac{1}{m\omega_0}[\hat{p}, \hat{x}]\right),$$

or

$$\hat{a}^{+}\hat{a} = \frac{1}{\hbar\omega_0}\left(\hat{H} - \frac{1}{2}\hbar\omega_0\right),$$

we obtaine the Hamiltonian as

$$\hat{H} = \hbar\omega_0\left(\hat{N} + \frac{1}{2}\right).$$

where

$$\hat{N} = \hat{a}^{+}\hat{a}.$$

The operator $\hat{N}$ is Hermitian since

$$\hat{N}^{+} = \left(\hat{a}^{+}\hat{a}\right)^{+} = \hat{a}^{+}\hat{a} = \hat{N}$$

The eigenvectors of $\hat{H}$ are those of $\hat{N}$, and vice versa since $[\hat{H}, \hat{N}] = 0$.

6.8 Annihilation operator $\hat{a}$ and creation operator $\hat{a}^{+}$

$$[\hat{N},\hat{a}] = \left[\hat{a}^{+}\hat{a},\hat{a}\right] = \hat{a}^{+}\hat{a}\hat{a} - \hat{a}\hat{a}^{+}\hat{a} = \left[\hat{a}^{+},\hat{a}\right]\hat{a} = -\hat{a} \,,$$

$$[\hat{N},\hat{a}^{+}] = \left[\hat{a}^{+}\hat{a},\hat{a}^{+}\right] = \hat{a}^{+}\hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a}^{+}\hat{a} = \hat{a}^{+}\left[\hat{a},\hat{a}^{+}\right] = \hat{a}^{+} \,.$$

Thus we have the relations

$$[\hat{N},\hat{a}] = -\hat{a} \,,$$

and

$$[\hat{N},\hat{a}^{+}] = \hat{a}^{+} \,.$$

From the relation $[\hat{N},\hat{a}]\left|n\right\rangle = -\hat{a}\left|n\right\rangle$,

$$(\hat{N}\hat{a} - \hat{a}\hat{N})\left|n\right\rangle = -\hat{a}\left|n\right\rangle ,$$

or

$$\hat{N}(\hat{a}\left|n\right\rangle) = (n-1)\hat{a}\left|n\right\rangle ,$$

which implies that $\hat{a}\left|n\right\rangle$ is the eigenket of $\hat{N}$ with the eigenvalue (n-1),

$$\hat{a}\left|n\right\rangle \approx \left|n-1\right\rangle .$$

Similarly, from the relation $[\hat{N},\hat{a}^{+}]\left|n\right\rangle = \hat{a}^{+}\left|n\right\rangle$, we have

$$(\hat{N}\hat{a} - \hat{a}\hat{N})\left|n\right\rangle = -\hat{a}\left|n\right\rangle ,$$

or

$$\hat{N}(\hat{a}^{+}\left|n\right\rangle) = (n+1)\hat{a}^{+}\left|n\right\rangle ,$$

which implies that $\hat{a}^{+}\left|n\right\rangle$ is the eigenket of $\hat{N}$ with the eigenvalue (n+1),

$$\hat{a}^{+}\left|n\right\rangle \approx \left|n+1\right\rangle .$$

Now we need to show that n should be either zero or positive integers: n = 0, 1, 2, 3,….

We note that

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = n\langle n|n\rangle \geq 0$$

$$\langle n|\hat{a}\hat{a}^{+}|n\rangle = \langle n|\hat{a}^{+}\hat{a}+1|n\rangle = (n+1)\langle n|n\rangle \geq 0$$

The norm of a ket vector is non-negative and the vanishing of the norm is a necessary and sufficient condition for the vanishing of the ket vector. In other words, $n \geq 0$. If n = 0, $\hat{a}|n\rangle = 0$. If $n \neq 0$, $\hat{a}|n\rangle$ is a nonzero ket vector of norm $n\langle n|n\rangle$. If n>0, one successively forms the set of eigenkets,

$\hat{a}|n\rangle, \hat{a}^{2}|n\rangle, \hat{a}^{3}|n\rangle, \ldots.\ \hat{a}^{p}|n\rangle,$, belonging to the eigenvalues, n-1, n-2, n-3,….., n-p,

This set is certainly limited since the eigenvalues of $\hat{N}$ have a lower limit of zero. In other words, the eigenket $\hat{a}^{p}|n\rangle \approx |n-p\rangle$, or n-p = 0. Thus n should be a positive integer. Similarly, one successively forms the set of eigenkets,

$\hat{a}^{+}|n\rangle, \hat{a}^{+^{2}}|n\rangle, \hat{a}^{+^{3}}|n\rangle, \ldots.\ \hat{a}^{+^{p}}|n\rangle$, belonging to the eigenvalues, n+1, n+2, n+3,….., n+p,

Thus the eigenvalues are either zero or positive integers: n = 0, 1, 2, 3, 4, .

(A) The properties of $\hat{a}^{+}$ and $\hat{a}$

(i) $\hat{a}|0\rangle = 0$

since $\langle 0|\hat{a}^{+}\hat{a}|0\rangle = 0$.

(ii) $\hat{a}^{+}|n\rangle = \sqrt{n+1}|n+1\rangle$,

$$[\hat{N}, \hat{a}^{+}]|n\rangle = \hat{a}^{+}|n\rangle,$$

$$\hat{N}\hat{a}^{+}|n\rangle = \hat{a}^{+}\hat{N}|n\rangle + \hat{a}^{+}|n\rangle = (n+1)\hat{a}^{+}|n\rangle.$$

$\hat{a}^{+}|n\rangle$ is an eigenket of $\hat{N}$ with the eigenvalue (n + 1).

Then

$$\hat{a}^{+}|n\rangle = c|n+1\rangle.$$

Since

$$\langle n|\hat{a}\hat{a}^{+}|n\rangle = |c|^2 \langle n+1|n+1\rangle = |c|^2 ,$$

or

$$\langle n|\hat{a}^{+}\hat{a}+1|n\rangle = n+1 = |c|^2 ,$$

or

$$|c| = \sqrt{n+1} .$$

(iii) $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle ,$

$$[\hat{N},\hat{a}]|n\rangle = -\hat{a}|n\rangle ,$$

$$\hat{N}\hat{a}|n\rangle = \hat{a}\hat{N}|n\rangle - \hat{a}|n\rangle = (n-1)\hat{a}|n\rangle .$$

$\hat{a}|n\rangle$ is an eigenket of $\hat{N}$ with the eigenvalue (n - 1). Then we have

$$\hat{a}|n\rangle = c|n-1\rangle .$$

Since

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = |c|^2 \langle n-1|n-1\rangle = |c|^2 = n ,$$

or

$$|c| = \sqrt{n} .$$

(B) Basis vectors in terms of $|0\rangle$

We use the relation

$$|1\rangle = \hat{a}^{+}|0\rangle$$

$$|2\rangle = \frac{1}{\sqrt{2}}\hat{a}^{+}|1\rangle = \frac{1}{\sqrt{2!}}(\hat{a}^{+})^2|0\rangle$$

$$|3\rangle = \frac{1}{\sqrt{3}}\hat{a}^{+}|2\rangle = \frac{1}{\sqrt{3!}}(\hat{a}^{+})^3|0\rangle$$

$$|n\rangle = \frac{1}{\sqrt{n}}\hat{a}^{+}|n-1\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^{+}\right)^{n}|0\rangle$$

6.9 Matrices

The expression for $\hat{x}|n\rangle$ and $\hat{p}|n\rangle$

$$\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\hat{a}+\hat{a}^{+}\right)|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\sqrt{n+1}|n+1\rangle + \sqrt{n}|n-1\rangle\right)$$

$$\hat{p}|n\rangle = \sqrt{\frac{m\hbar\omega_0}{2}}i\left(\hat{a}^{+}-\hat{a}\right)|n\rangle = \sqrt{\frac{m\hbar\omega_0}{2}}i\left(\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle\right)$$

Therefore the matrix elements of $\hat{a}$, $\hat{a}^{+}$, $\hat{x}$, and $\hat{p}$ operators in the $\{|n\rangle\}$ representation are as follows.

$$\langle n'|\hat{a}|n\rangle = \sqrt{n}\delta_{n',n-1},$$

$$\langle n'|\hat{a}^{+}|n\rangle = \sqrt{n+1}\delta_{n',n+1},$$

$$\langle n'|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega_0}}\left(\sqrt{n+1}\delta_{n',n+1} + \sqrt{n}\delta_{n',n-1}\right),$$

$$\langle n'|\hat{p}|n\rangle = i\sqrt{\frac{m\hbar\omega_0}{2}}\left(\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}\right),$$

$$\hat{H} = \hbar\omega\begin{pmatrix} 1/2 & 0 & \cdots & 0 & \cdots \\ 0 & 3/2 & & & \\ \vdots & & \ddots & & \\ 0 & & & (2n+1)/2 & \\ \vdots & & & & \ddots \end{pmatrix},$$

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix},$$

$$\hat{p} = \frac{m\omega_0}{\sqrt{2}i\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & -\sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix},$$

$$\hat{a} = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & \vdots & & & \end{pmatrix},$$

$$\hat{a}^{+} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix},$$

$$
\hat{N} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \\ \sqrt{1} & 0 & 0 & 0 & 0 & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{2} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \\ & & \vdots & & & \end{pmatrix}
$$

$$
= \begin{pmatrix} 0 & 0 & 0 & 0 & & & \\ 0 & 1 & 0 & 0 & & & \\ 0 & 0 & 2 & 0 & & & \\ 0 & 0 & 0 & 3 & & & \\ & & & & \ddots & & \\ & & & & & n & \\ & & & & & & \ddots \end{pmatrix},
$$

Mean values and root-mean-square deviations of $\hat{x}$ and $\hat{p}$ in the state $|n\rangle$.

$$
\langle n|\hat{x}|n\rangle = 0,
$$

$$
\langle n|\hat{p}|n\rangle = 0,
$$

$$
(\Delta x)^2 = \langle n|\hat{x}^2|n\rangle = \left(n + \frac{1}{2}\right)\frac{\hbar}{m\omega_0},
$$

$$
(\Delta p)^2 = \langle n|\hat{p}^2|n\rangle = \left(n + \frac{1}{2}\right)m\hbar\omega_0.
$$

The product $\Delta x \Delta p$ is evaluated as

$$
\Delta x \Delta p = \left(n + \frac{1}{2}\right)\hbar \ge \frac{1}{2}\hbar \qquad \text{(Heisenberg's principle of uncertainty)}
$$

Note that

$$
\hat{x}^2 = \frac{\hbar}{2m\omega_0}\left(\hat{a}^+ + \hat{a}\right)\left(\hat{a}^+ + \hat{a}\right) = \frac{\hbar}{2m\omega_0}\left(\hat{a}^+\hat{a}^+ + \hat{a}\hat{a} + \hat{a}^+\hat{a} + \hat{a}\hat{a}^+\right),
$$

$$
\hat{p}^2 = \frac{m\hbar\omega_0}{2}\left(\hat{a}^+ - \hat{a}\right)\left(\hat{a}^+ - \hat{a}\right) = \frac{m\hbar\omega_0}{2}\left(\hat{a}^+\hat{a}^+ + \hat{a}\hat{a} - \hat{a}^+\hat{a} - \hat{a}\hat{a}^+\right),
$$

and

$$\langle n|(\hat{a}^{+})^{2}|n\rangle = 0\,,$$

$$\langle n|\hat{a}^{2}|n\rangle = 0\,,$$

$$\langle n|\hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+}|n\rangle = \langle n|2\hat{a}^{+}\hat{a} + 1|n\rangle = 2n + 1\,.$$

Mean potential energy

$$\langle V\rangle = \frac{1}{2}m\omega^{2}\langle n|\hat{x}^{2}|n\rangle = \frac{1}{2}m\omega^{2}(\Delta x)^{2} = \frac{1}{2}\varepsilon_{n}\,.$$

Mean kinetic energy

$$\langle K\rangle = \frac{1}{2m}\langle n|\hat{p}^{2}|n\rangle = \frac{1}{2m}(\Delta p)^{2} = \frac{1}{2}\varepsilon_{n}\,.$$

Thus we have

$$\langle V\rangle = \langle K\rangle\,.$$

6.10 Representation of the state |*n*> under the basis of |*x*> and |ξ>

We assume that

$$\xi = \beta x.$$

where ξ is a dimensionless quantity. Then we have

$$\langle \xi|\xi'\rangle = \delta(\xi - \xi') = \delta[\beta(x - x')] = \frac{1}{\beta}\delta(x - x') = \frac{1}{\beta}\langle x|x'\rangle\,,$$

using the property of the Dirac delta function (which will be discussed later). This implies that

$$|\xi\rangle = \frac{1}{\sqrt{\beta}}|x\rangle\,.$$

Using this notation, the wave functions in the presentation of {|*x*>} and {|ξ>} can be expressed by

$$\varphi_n(x) = \langle x|n\rangle = \sqrt{\beta}\langle\xi|n\rangle = \sqrt{\beta}\varphi_n(\xi).$$

We also note that

$$\hat{a} = \frac{1}{\sqrt{2}}(\xi + \frac{\partial}{\partial\xi}),$$

and

$$\hat{a}^+ = \frac{1}{\sqrt{2}}(\xi - \frac{\partial}{\partial\xi}).$$

6.11 Solution for the wave function $\varphi_n(\xi)$

We start with

$$\hat{a}|0\rangle = 0,$$

or

$$\frac{\beta}{\sqrt{2}}\left(\hat{x} + i\frac{\hat{p}}{m\omega_0}\right)|0\rangle = 0,$$

with

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

$$\langle x|\frac{\beta}{\sqrt{2}}\left(\hat{x} + i\frac{\hat{p}}{m\omega_0}\right)|0\rangle = 0,$$

$$x\langle x|0\rangle + \frac{i}{m\omega_0}\langle x|\hat{p}|0\rangle = 0.$$

We assume that

$$\varphi_0(x) = \langle x|0\rangle.$$

Then we have

$$\beta x\varphi_0(x) + \frac{\hbar}{m\omega 0}\beta\frac{\partial}{\partial x}\varphi_0(x) = 0,$$

or

$$\beta x\varphi_0(x) + \frac{1}{\beta}\frac{\partial}{\partial x}\varphi_0(x) = 0\,.$$

Since $\frac{\partial}{\partial x} = \frac{\partial\xi}{\partial x}\frac{\partial}{\partial\xi} = \beta\frac{\partial}{\partial\xi}$, we get

$$(\xi + \frac{\partial}{\partial\xi})\varphi_0(\xi) = 0\,,$$

or

$$\frac{\partial}{\partial\xi}\varphi_0(\xi) = -\xi\varphi_0(\xi)\,,$$

where

$$\varphi_0(\xi) = \langle\xi|0\rangle\,.$$

The wave function $\varphi_0(\xi)$ can be obtained as

$$\varphi_0(\xi) = A_0 e^{-\xi^2/2}\,.$$

The condition of normalization given by

$$1 = \int_{-\infty}^{\infty}|\varphi_0(\xi)|^2 d\xi = |A_0|^2\int_{-\infty}^{\infty}e^{-\xi^2}d\xi = |A_0|^2\pi$$

leads to $A_0 = \pi^{-1/4}$. Here we assume that A_0 is real. then we have

$$\varphi_0(\xi) = \pi^{-1/4}e^{-\xi^2/2}\,.$$

The wave function $\varphi_n(x)$ is given by

$$\begin{aligned}\varphi_n(x) = \langle x|n\rangle &= \frac{1}{\sqrt{n!}}\langle x|(\hat{a}^+)^n|0\rangle = \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\beta^n\langle x|\left(\hat{x} - \frac{i\hat{p}}{m\omega_0}\right)^n|0\rangle \\ &= \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}\beta^n\left(x - \frac{\hbar}{m\omega_0}\frac{\partial}{\partial x}\right)^n\varphi_0(x)\end{aligned}$$

(Note)) In general, one can use the formula,

$$\langle x|f(\hat{x},\hat{p})|n\rangle = f(x,\frac{\hbar}{i}\frac{\partial}{\partial x})\langle x|n\rangle$$

Since

$$\varphi_n(\xi) = \frac{1}{\sqrt{\beta}}\varphi_n(x)$$

we have

$$\varphi_n(\xi) = \frac{1}{\sqrt{n!}}\frac{1}{\sqrt{2^n}}(\xi - \frac{\partial}{\partial\xi})^n\varphi_0(\xi)\,,$$

or

$$\varphi_n(\xi) = (\sqrt{\pi}\,2^n n!)^{-1/2}(\xi - \frac{\partial}{\partial\xi})^n e^{-\xi^2/2}\,.$$

Using the operator identity

$$\xi - \frac{\partial}{\partial\xi} = -e^{\xi^2/2}\frac{\partial}{\partial\xi}e^{-\xi^2/2}$$

$$(\xi - \frac{\partial}{\partial\xi})^2 = -e^{\xi^2/2}\frac{\partial}{\partial\xi}e^{-\xi^2/2}(-e^{\xi^2/2}\frac{\partial}{\partial\xi}e^{-\xi^2/2})$$
$$= (-1)^2 e^{\xi^2/2}\frac{\partial^2}{\partial\xi^2}e^{-\xi^2/2}$$

....

in general

$$(\xi - \frac{\partial}{\partial\xi})^n = (-1)^n e^{\xi^2/2}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2/2}\,.$$

Then we obtain

$$\varphi_n(\xi) = (\sqrt{\pi}\,2^n n!)^{-1/2}(-1)^n e^{\xi^2/2}\frac{\partial^n}{\partial\xi^n}e^{-\xi^2}\,.$$

Using the Hermite polynomial defined by

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2},$$

we have

$$\varphi_n(\xi) = (\sqrt{\pi} 2^n n!)^{-1/2} e^{-\xi^2/2} H_n(\xi).$$

((Note))

$$(\xi - \frac{\partial}{\partial \xi})^n e^{-\xi^2/2} = (-1)^n e^{\xi^2/2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2}$$

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2} = e^{\xi^2/2} (\xi - \frac{\partial}{\partial \xi})^n e^{-\xi^2/2}$$

The Hermite polynomial satisifies the differential equation

$$(\frac{d^2}{d\xi^2} - 2\xi \frac{d}{d\xi} + 2n) H_n(\xi) = 0.$$

6.12 A few auxiliary mathematical relations

(a)

$$\hat{H} = \hbar\omega_0 \left(\hat{a}^+ \hat{a} + \frac{1}{2} \hat{1} \right)$$

$$\hat{a}^+ \hat{a} = \frac{\beta^2}{2} \left(\hat{x} - \frac{i\hat{p}}{m\omega_0} \right) \left(\hat{x} + \frac{i\hat{p}}{m\omega_0} \right)$$

$$\langle x | \hat{H} | n \rangle = \hbar\omega_0 \langle x | \left(\hat{a}^+ \hat{a} + \frac{1}{2} \hat{1} \right) | n \rangle = \hbar\omega_0 (n + \frac{1}{2}) \langle x | n \rangle$$

or

$$\langle x | \left(\hat{a}^+ \hat{a} + \frac{1}{2} \hat{1} \right) | n \rangle = \frac{\beta^2}{2} \left(x - \frac{\hbar}{m\omega_0} \frac{\partial}{\partial x} \right) \left(x + \frac{\hbar}{m\omega_0} \frac{\partial}{\partial x} \right) \langle x | n \rangle = (n + \frac{1}{2}) \langle x | n \rangle$$

Here we use $\xi = \beta x$, $|\xi\rangle = \frac{1}{\sqrt{\beta}} |x\rangle$, and $\varphi_n(\xi) = \langle \xi | n \rangle$

$$\left(\xi-\frac{\partial}{\partial\xi}\right)\left(\xi+\frac{\partial}{\partial\xi}\right)\varphi_n(\xi)=(2n+1)\varphi_n(\xi)$$

where

$$\varphi_n(\xi)=(\sqrt{\pi}\,2^n n!)^{-1/2}e^{-\xi^2/2}H_n(\xi)$$

or

$$\left(\xi-\frac{\partial}{\partial\xi}\right)\left(\xi+\frac{\partial}{\partial\xi}\right)e^{-\xi^2/2}H_n(\xi)=(2n+1)e^{-\xi^2/2}H_n(\xi).$$

(b)

$$\hat{a}^+|n\rangle=\sqrt{n+1}|n+1\rangle,$$

$$\hat{a}^+=\frac{\beta}{\sqrt{2}}\left(\hat{x}-\frac{i\hat{p}}{m\omega_0}\right),$$

$$\langle x|\hat{a}^+|n\rangle=\sqrt{n+1}\langle x|n+1\rangle,$$

or

$$\frac{\beta}{\sqrt{2}}(x-\frac{\hbar}{m\omega_0}\frac{\partial}{\partial x})\langle x|n\rangle=\sqrt{n+1}\langle x|n+1\rangle,$$

or

$$(\xi-\frac{\partial}{\partial\xi})\langle\xi|n\rangle=\sqrt{2(n+1)}\langle\xi|n+1\rangle. \quad \text{(Arfken p.826)}$$

(c)
Similarly we have

$$(\xi+\frac{\partial}{\partial\xi})\langle\xi|n\rangle=\sqrt{2n}\langle\xi|n-1\rangle, \qquad \text{(Arfken p.826)}$$

from the relation, $\hat{a}|n\rangle=\sqrt{n}|n-1\rangle$.

6.13 Mathematica

Using the Mathematica ,we make the following calculations,

1. Derivation of the Hermite differential equation

$$\hat{a} = \frac{1}{\sqrt{2}}(\xi + \frac{\partial}{\partial \xi}),$$

and

$$\hat{a}^{+} = \frac{1}{\sqrt{2}}(\xi - \frac{\partial}{\partial \xi}).$$

$$\hat{a}^{+}\hat{a}\langle \xi | n \rangle = n \langle \xi | n \rangle$$

2. Hermite polynomials

$$H_n(\xi) = e^{\xi^2/2}(\xi - \frac{\partial}{\partial \xi})^n e^{-\xi^2/2}$$

with

$$(\xi - \frac{\partial}{\partial \xi})^n = (-1)^n e^{\xi^2/2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2/2}$$

3. Wavefunctions

$$\varphi_n(\xi) = (\sqrt{\pi} 2^n n!)^{-1/2} e^{-\xi^2/2} H_n(\xi) = (\sqrt{\pi} 2^n n!)^{-1/2} (\xi - \frac{\partial}{\partial \xi})^n e^{-\xi^2/2}$$

((**Mathematica**))

Creation and annihilation operators : differential form

```
Clear["Global`*"];
```

$$CR := \frac{1}{\sqrt{2}} (\xi \# - D[\#, \xi]) \&;$$

$$AN := \frac{1}{\sqrt{2}} (\xi \# + D[\#, \xi]) \&;$$

```
eq1 = CR[AN[ψ[ξ]]] == n ψ[ξ] // Simplify
```

$$\psi[\xi] + 2\, n\, \psi[\xi] + \psi''[\xi] == \xi^2\, \psi[\xi]$$

$$\text{srule} = \left\{\psi \to \left(\text{Exp}\left[-\frac{\#^2}{2}\right] H[\#] \,\&\right)\right\};$$

```
eq11 = eq1 /. srule // Simplify
```

$$e^{-\frac{\xi^2}{2}} \left(2\, n\, H[\xi] - 2\, \xi\, H'[\xi] + H''[\xi]\right) == 0$$

```
DSolve[eq11, H[ξ], ξ]
```

$$\left\{\left\{H[\xi] \to C[1]\, \text{HermiteH}[n, \xi] + C[2]\, \text{Hypergeometric1F1}\left[-\frac{n}{2}, \frac{1}{2}, \xi^2\right]\right\}\right\}$$

```
φ[n_, ξ_] := π^-1/4 (2^n n!)^-1/2 Exp[-ξ^2/2] HermiteH[n, ξ] // Simplify;

φ0[ξ_] := π^-1/4 Exp[-ξ^2/2];

ψ[n_, ξ_] := 1/Sqrt[n!] Nest[CR, φ0[ξ], n] // FullSimplify

Table[{n, ψ[n, ξ], φ[n, ξ], ψ[n, ξ] - φ[n, ξ] }, {n, 0, 6}] //
  Simplify // TableForm
```

0	$\frac{e^{-\frac{\xi^2}{2}}}{\pi^{1/4}}$	$\frac{e^{-\frac{\xi^2}{2}}}{\pi^{1/4}}$	0
1	$\frac{\sqrt{2}\, e^{-\frac{\xi^2}{2}}\, \xi}{\pi^{1/4}}$	$\frac{\sqrt{2}\, e^{-\frac{\xi^2}{2}}\, \xi}{\pi^{1/4}}$	0
2	$\frac{e^{-\frac{\xi^2}{2}} \left(-1+2\,\xi^2\right)}{\sqrt{2}\, \pi^{1/4}}$	$\frac{e^{-\frac{\xi^2}{2}} \left(-1+2\,\xi^2\right)}{\sqrt{2}\, \pi^{1/4}}$	0
3	$\frac{e^{-\frac{\xi^2}{2}}\, \xi \left(-3+2\,\xi^2\right)}{\sqrt{3}\, \pi^{1/4}}$	$\frac{e^{-\frac{\xi^2}{2}}\, \xi \left(-3+2\,\xi^2\right)}{\sqrt{3}\, \pi^{1/4}}$	0
4	$\frac{e^{-\frac{\xi^2}{2}} \left(3+4\,\xi^2 \left(-3+\xi^2\right)\right)}{2\sqrt{6}\, \pi^{1/4}}$	$\frac{e^{-\frac{\xi^2}{2}} \left(3-12\,\xi^2+4\,\xi^4\right)}{2\sqrt{6}\, \pi^{1/4}}$	0
5	$\frac{e^{-\frac{\xi^2}{2}}\, \xi \left(15+4\,\xi^2 \left(-5+\xi^2\right)\right)}{2\sqrt{15}\, \pi^{1/4}}$	$\frac{e^{-\frac{\xi^2}{2}}\, \xi \left(15-20\,\xi^2+4\,\xi^4\right)}{2\sqrt{15}\, \pi^{1/4}}$	0
6	$\frac{e^{-\frac{\xi^2}{2}} \left(-15+90\,\xi^2-60\,\xi^4+8\,\xi^6\right)}{12\sqrt{5}\, \pi^{1/4}}$	$\frac{e^{-\frac{\xi^2}{2}} \left(-15+90\,\xi^2-60\,\xi^4+8\,\xi^6\right)}{12\sqrt{5}\, \pi^{1/4}}$	0

6.14 Schrödinger equation

We consider the Schrödinger equation defined by

$$\langle x|\hat{H}|n\rangle = \varepsilon_n \langle x|n\rangle ,$$

or

$$\langle x|\frac{1}{2m}\hat{p}^2 + \frac{m\omega_0^2}{2}\hat{x}^2|n\rangle = \varepsilon_n \langle x|n\rangle ,$$

or

$$(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega_0{}^2}{2}x^2)\varphi_n(x) = \varepsilon_n \varphi_n(x) ,$$

with

$$\varphi_n(x) = \langle x|n\rangle .$$

Here we use ξ instead of x;

$$\xi = \beta x ,$$

with

$$\beta = \sqrt{\frac{m\omega_0}{\hbar}} . \qquad \text{(unit: cm}^{-1}\text{)}.$$

Using the relations given by

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} = \beta \frac{\partial}{\partial \xi} ,$$

and

$$\frac{\partial^2}{\partial x^2} = \beta \frac{\partial}{\partial \xi}(\beta \frac{\partial}{\partial \xi}) = \beta^2 \frac{\partial^2}{\partial \xi^2} ,$$

we get

$$(-\frac{\hbar^2}{2m}\beta^2 \frac{d^2}{d\xi^2} + \frac{m\omega_0{}^2}{2}\frac{\xi^2}{\beta^2})\langle \xi|n\rangle = \varepsilon_n \langle \xi|n\rangle ,$$

or

$$(-\frac{\hbar\omega_0}{2}\frac{d^2}{d\xi^2} + \frac{\hbar\omega_0}{2}\xi^2)\langle \xi|n\rangle = \hbar\omega_0(n + \frac{1}{2})\langle \xi|n\rangle ,$$

or

$$(\frac{d^2}{d\xi^2} - \xi^2 + 2n + 1)\varphi_n(\xi) = 0 ,$$

with

$$\varphi_n(\xi) = \langle \xi|n\rangle = \frac{1}{\sqrt{\beta}}\varphi_n(x) .$$

6.15 Sturm-Liouville type differential equation

We put

$$\varphi_n(\xi) = e^{-\xi^2/2} u_n(\xi),$$

with $u_n(\xi) = H_n(\xi)$: Hermite polynomials. H_n(x) satisfies the differential equation.

$$H_n''(\xi) - 2\xi H_n'(\xi) + 2nH_n(\xi) = 0. \qquad (1)$$

Equation (1) is not a Sturm-Liouville type differential equation. In order to get the Sturm-Liouville type diffrential equation, we multiply the weight function $w(\xi)$,

$$w(\xi)H_n''(\xi) - 2\xi w(\xi)H_n'(\xi) + 2nw(\xi)H_n(\xi) = 0.$$

The weight function should be determined such that

$$w(\xi)H_n''(\xi) - 2\xi w(\xi)H_n'(\xi) = \frac{d}{d\xi}[w(\xi)H_n'(\xi)].$$

or

$$w'(\xi) = -2\xi w(\xi),$$

$$w(\xi) = \exp(-\xi^2).$$

Then we have

$$L[H_n] + \lambda_n w(\xi)H_n(\xi) = 0,$$

with

$$L[H_n] = \frac{d}{d\xi}[w(\xi)H_n'(\xi)].$$

The weight function is given by

$$w(\xi) = \exp(-\xi^2).$$

The eigenvalue is

$$\lambda_n = 2n.$$

6.16 Orthogonality

We consider the eigenfunctions,

$$L[H_n] + 2n\exp(-\xi^2)H_n = 0\,,$$

and

$$L[H_m] + 2m\exp(-\xi^2)H_m = 0\,.$$

We show that operator $\hat{L}$ is a Hermitian.

$$\int_{-\infty}^{\infty} H_m{}^* L[H_n] d\xi = \int_{-\infty}^{\infty} H_n L[H_m{}^*] d\xi\,.$$

((**Proof**))

$$\langle H_m|\hat{L}|H_n\rangle = \langle H_n|\hat{L}^+|H_m\rangle^*$$

$$\begin{aligned}
\langle H_m|\hat{L}|H_n\rangle &= \int_{-\infty}^{\infty} H_m{}^* L[H_n] d\xi = \int_{-\infty}^{\infty} H_m{}^* \frac{d}{d\xi}[w(\xi)H_n'(\xi)] d\xi \\
&= -\int_{-\infty}^{\infty} (\frac{d}{d\xi} H_m{}^*)[w(\xi)H_n'(\xi)] d\xi = \int_{-\infty}^{\infty} \frac{d}{d\xi}(w(\xi)\frac{d}{d\xi} H_m{}^*) H_n(\xi) d\xi \\
&= \int_{-\infty}^{\infty} H_n L[H_m{}^*] d\xi = \int_{-\infty}^{\infty} H_n L[H_m]^* d\xi \\
&= \left(\int_{-\infty}^{\infty} H_n{}^* L[H_m] d\xi\right)^* = \langle H_n|\hat{L}|H_m\rangle^*
\end{aligned}$$

In other words, we get

$$\hat{L}^+ = \hat{L}\,. \qquad \text{(Hermitian operator)}$$

Then we have

$$\int_{-\infty}^{\infty} H_m{}^*[-2nw(\xi)]H_n(\xi) d\xi = \left(\int_{-\infty}^{\infty} H_n{}^*[-2mw(\xi)]H_m(\xi) d\xi\right)^*,$$

or

$$(n-m)\int_{-\infty}^{\infty} H_m^{*} w(\xi)]H_n(\xi)d\xi = 0\,,$$

or

$$(n-m)\int_{-\infty}^{\infty} H_m^{*} e^{-\xi^2} H_n(\xi)d\xi = 0\,,$$

If $n \neq m$,

$$\int_{-\infty}^{\infty} H_m^{*}(\xi) e^{-\xi^2} H_n(\xi)d\xi = 0\,,$$

or

$$\int_{-\infty}^{\infty} H_m(\xi) e^{-\xi^2} H_n(\xi)d\xi = 0\,.$$

since $H_n(\xi)$ is a real function.

6.17 Normalization

Here we define the wave function as

$$\varphi_n(\xi) = (\sqrt{\pi}\,2^n n!)^{-1/2} e^{-\xi^2/2} H_n(\xi)\,,$$

where

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2}\,.$$

We show that $\varphi_n(\xi)$ is the normalized wave function;

$$\int_{-\infty}^{\infty} \varphi_n^{*}(\xi)\varphi_n(\xi)d\xi = 1\,,$$

or

$$\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi)H_n(\xi)d\xi = 2^n n!\sqrt{\pi}\,.$$

((Proof))

$$\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi) H_n(\xi) d\xi = (-1)^n \int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi) [e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2}] d\xi =$$

$$= (-1)^n \int_{-\infty}^{\infty} H_n(\xi) \frac{\partial^n}{\partial \xi^n} e^{-\xi^2} d\xi = (-1)^n (-1)^n \int_{-\infty}^{\infty} e^{-\xi^2} \frac{\partial^n}{\partial \xi^n} H_n(\xi) d\xi$$

$H_n(\xi)$ is the Hermite polynomial and is a function of ξ. The highest power is ξ^n and the coefficient for the power ξ^n is 2^n.

$$\frac{\partial^n}{\partial \xi^n} H_n(\xi) = 2^n n!.$$

Thus we have

$$\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi) H_n(\xi) d\xi = 2^n n! \int_{-\infty}^{\infty} e^{-\xi^2} d\xi = 2^n n! \sqrt{\pi} ,$$

or

$$\int_{-\infty}^{\infty} \varphi_n^*(\xi) \varphi_n(\xi) d\xi = 1 .$$

6.18 Dirac delta function

An arbitrary function $\psi(\xi)$ can be expanded in terms of complete set $\{u_n(\xi)\}$ as

$$\psi(\xi) = \sum_n a_n u_n(\xi) .$$

Note that

$$\begin{aligned}
\int_a^b u_n^*(\varsigma) w(\varsigma) \psi(\varsigma) d\varsigma &= \int_a^b u_n^*(\varsigma) w(\varsigma) \sum_m a_m u_m(\varsigma) d\varsigma \\
&= \sum_m a_m \int_a^b u_n^*(\varsigma) w(\varsigma) u_m(\varsigma) d\varsigma \\
&= \sum_m a_m \delta_{nm} = a_n
\end{aligned}$$

where

$$\int_a^b u_n^*(\varsigma)w(\varsigma)u_m(\varsigma)d\varsigma = \delta_{nm} .$$

Then we have

$$\psi(\xi) = \sum_n u_n(\xi)\int_a^b u_n^*(\varsigma)w(\varsigma)\psi(\varsigma)d\varsigma = \int_a^b \sum_n [u_n(\xi)w(\varsigma)u_n^*(\varsigma)]\psi(\varsigma)d\varsigma .$$

Since $\psi(\xi)$ is an arbitrary function, one can say that

$$\sum_n [u_n(\xi)w(\varsigma)u_n^*(\varsigma)] = w(\varsigma)\sum_n [u_n(\xi)u_n^*(\varsigma)] = \delta(\varsigma - \xi) .$$

Then we have

$$\psi(\xi) = \int_a^b \delta(\varsigma - \xi)\psi(\varsigma)d\varsigma ,$$

from the property of the delta function.

In the case of the Hermite differential equation,

$$u_n(\xi) = (2^n n!\sqrt{\pi})^{-1/2} H_n(\xi) ,$$

with

$$w(\xi) = e^{-\xi^2} ,$$

and

$$\int_{-\infty}^{\infty} e^{-\xi^2} u_n^{\ *}(\xi)u_n(\xi)d\xi = (2^n n!\sqrt{\pi})^{-1} \int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi)H_n(\xi)d\xi = 1 .$$

6.19 Dirac function by Hermite polynomials

The Dirac delta function can be formed using the Hermite polynomials.

$$\begin{aligned}\delta(\varsigma - \xi) &= w(\varsigma)\sum_n [u_n(\xi)u_n^*(\varsigma)] \\ &= e^{-\varsigma^2} \sum_n \frac{H_n(\xi)H_n(\varsigma)}{2^n n!\sqrt{\pi}}\end{aligned}$$

((**Mathematica**))

```
Clear["Global`*"]

f[x_, k_] :=
 Exp[-x^2]
  Sum[(HermiteH[n, 0] HermiteH[n, x])/(2^n n! Sqrt[π]),
   {n, 0, k}]

pl1 =
  Plot[
   Evaluate[Table[f[x, k],
     {k, 50, 250, 50}]], {x, -1, 1},
   PlotRange → All,
   PlotStyle → Table[{Hue[0.15 i], Thick},
     {i, 0, 10}],
   AxesLabel → {"ξ", "f(ξ)"}];

g1 = Graphics[
   {Text[Style["n=50", Black, 12],
     {0, 3}],
    Text[Style["n=100", Black, 12],
     {0, 4.5}],
    Text[Style["n=250", Black, 12],
     {0, 7}]}];

Show[pl1, g1]
```

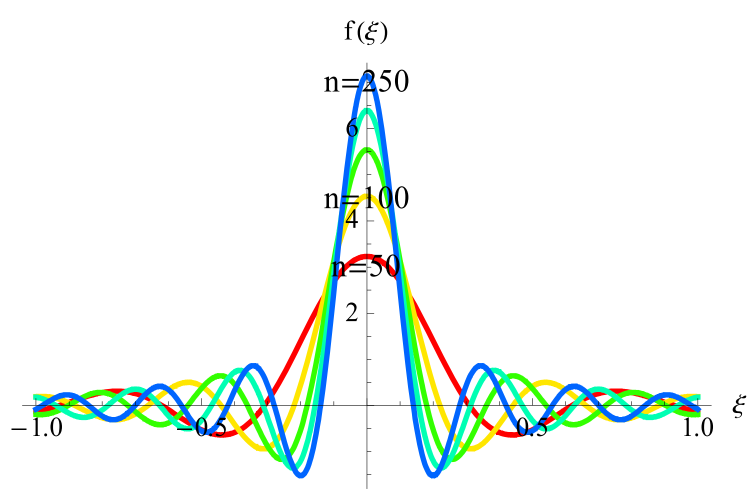


Fig.3

6.20 Plot of wave function

We make a plot of the function $|\varphi_n(\xi)|^2$ as a function of ξ for n = 0, 1, 2, 3,..., where

$$\varphi_n(\xi) = (\sqrt{\pi}\, 2^n n!)^{-1/2} e^{-\xi^2/2} H_n(\xi)$$

((**Mathematica**))

Simple Harmonics wave function: plot of φn[ξ]

```
conjugateRule = {Complex[re_, im_] :> Complex[re, -im]};
Unprotect[SuperStar];
SuperStar /: exp_* := exp /. conjugateRule;
Protect[SuperStar];

ψ[n_, ξ_] := 2^(-n/2) π^(-1/4) (n!)^(-1/2) Exp[-ξ^2/2] HermiteH[n, ξ];

Φ[n_, ξ_] := ψ[n, ξ]^2;

pt1[n_] := Plot[Evaluate[Φ[n, ξ]], {ξ, -6, 6},
  PlotLabel → {n}, PlotPoints → 100, PlotRange → All,
  DisplayFunction → Identity, Frame → True];
pt2 = Evaluate[Table[pt1[n], {n, 0, 8}]];
Show[GraphicsGrid[Partition[pt2, 2]]]
```

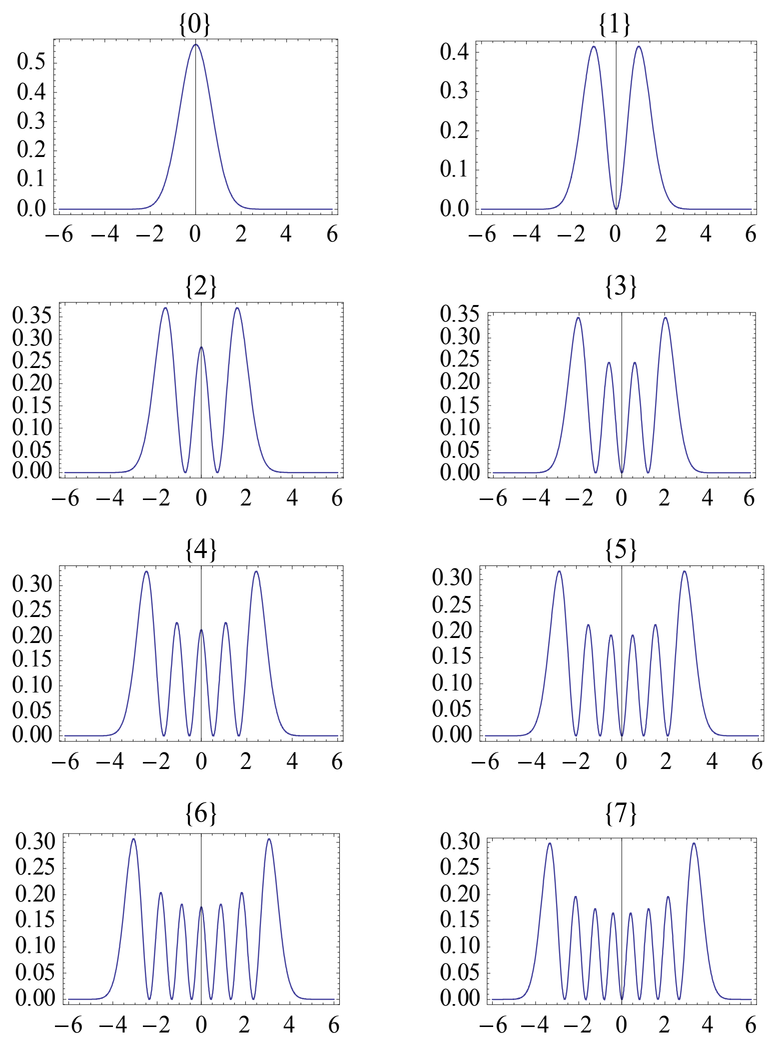


Fig.4

6.21 Classical limit: comparison with classical mechanics

Classical mechanics:

$$x = x_M \cos(\omega t - \varphi),$$

$$p = m\frac{dx}{dt} = -m\omega_0 x_M \sin(\omega t - \varphi),$$

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega_0^2 x^2 = \frac{1}{2}m\omega_0^2 x_M{}^2.$$

Comparison (classical mechanics and quantum mechanics)

We choose $\varphi = \pi/2$.

$$x = x_M \sin(\omega t),$$

$$p = m\frac{dx}{dt} = m\omega_0 x_M \cos(\omega t).$$

We define a classical "positional probability" as

$$W_{class}(x)dx = \frac{dt}{T},$$

where dt is the amount of time within dx and $T = 2\pi/\omega$.

$$dx = \omega x_M \cos(\omega t)dt = \omega x_M dt\sqrt{1-\sin^2(\omega t)} = \omega x_M dt\sqrt{1-(\frac{x}{x_M})^2},$$

since $\cos(\omega t) = \pm\sqrt{1-\sin^2(\omega t)} = \pm\sqrt{1-\left(\frac{x}{x_M}\right)^2}$,

$$W_{class}(x)\omega x_M dt\sqrt{1-(\frac{x}{x_M})^2} = \frac{dt}{T} = \frac{\omega dt}{2\pi},$$

or

$$W_{class}(x) = \frac{1}{2\pi}\frac{1}{x_M\sqrt{1-(\frac{x}{x_M})^2}}.$$

But this expression is not correct. Requiring that the total probability of finding the particle between $-x_M$ and x_M is unity determine the following correct expression

$$W_{class}(x) = \frac{1}{\pi} \frac{1}{x_M \sqrt{1-(\frac{x}{x_M})^2}} .$$

In fact

$$\int_{-x_M}^{x_M} W_{class}(x) dx = \int_{-x_M}^{x_M} \frac{1}{\pi} \frac{1}{x_M \sqrt{1-(\frac{x}{x_M})^2}} dx = 1 .$$

The reason for the factor 2 is as follows. The particle passes between x and x +dx twice during a period. We note that

$$x_M = \sqrt{\frac{2E}{m\omega_0^2}} = \sqrt{\frac{2\hbar\omega_0(n+\frac{1}{2})}{m\omega_0^2}} = \sqrt{2n+1}\sqrt{\frac{\hbar}{m\omega_0}} = \frac{\sqrt{2n+1}}{\beta} .$$

Since

$$W_{class}(\xi)d\xi = W_{class}(x)dx ,$$

or

$$W_{class}(\xi)d\xi = W_{class}(x)dx = W_{class}(x)\frac{1}{\beta}d\xi ,$$

or

$$W_{class}(\xi) = W_{class}(x)\frac{1}{\beta} ,$$

and

$$\xi = \beta x ,$$

$$W_{class}(\xi)d\xi = W_{class}(x)dx = \frac{\beta}{\pi\sqrt{2n+1}} \frac{1}{\sqrt{1-(\frac{\xi}{\sqrt{2n+1}})^2}} \frac{d\xi}{\beta} ,$$

$$W_{class}(\xi) = \frac{1}{\pi\sqrt{2n+1}} \frac{1}{\sqrt{1-(\frac{\xi}{\sqrt{2n+1}})^2}} .$$

Classical limit is given by

$$\frac{\xi^2}{2} = n + \frac{1}{2} .$$

The intercepts of the parabora ($\xi^2/2$) with horizontal lines (n+1/2) are the positions of the classical turning points. $W_{class}(\xi)$ is compared with $|\varphi_n(\xi)|^2$ (quantum mechanics).

$$W_{class}(\xi) = \lim_{n\to\infty} \frac{1}{2\varepsilon} \int_{\xi-\varepsilon}^{\xi+\varepsilon} |\varphi_n(\xi)^2| d\xi .$$

((**Mathematica**))

Classical limit of the simple harmonics

```
Clear["Global`*"]

φ[n_, ξ_] := 2^(-n/2) π^(-1/4) (n!)^(-1/2) Exp[-ξ^2/2] HermiteH[n, ξ];

plot1 = Plot[Table[φ[n, ξ]^2 + n + 0.5, {n, 0, 10}] // Evaluate,
   {ξ, -6, 6}, PlotStyle → Table[{Thick, Hue[0.07 i]}, {i, 0, 10}],
   Background → LightGray];

plot2 = Plot[ξ^2/2, {ξ, -6, 6}, PlotStyle → Thickness[0.01],
   Frame → True];

plot3 = Plot[Table[n + 0.5, {n, 0, 10}] // Evaluate, {ξ, -6, 6},
   PlotStyle → Table[{Thick, Hue[0.07 i]}, {i, 0, 10}]];

Show[plot1, plot2, plot3, PlotRange → {{-6, 6}, {0, 12}}]
```

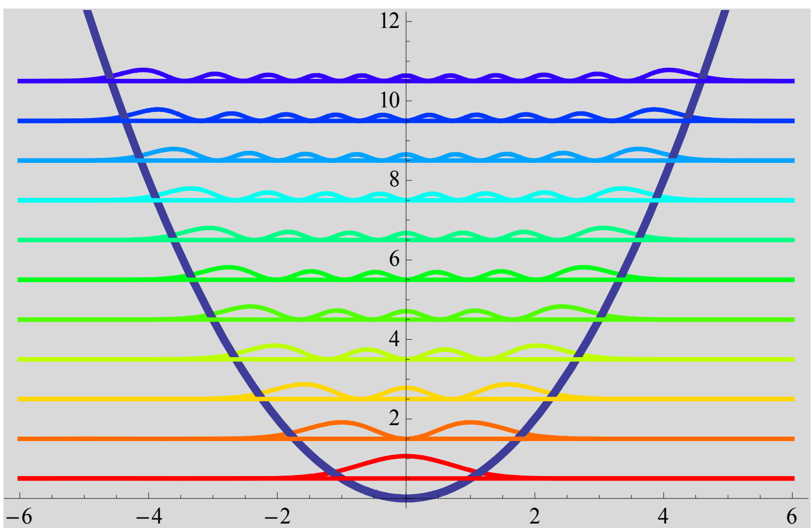
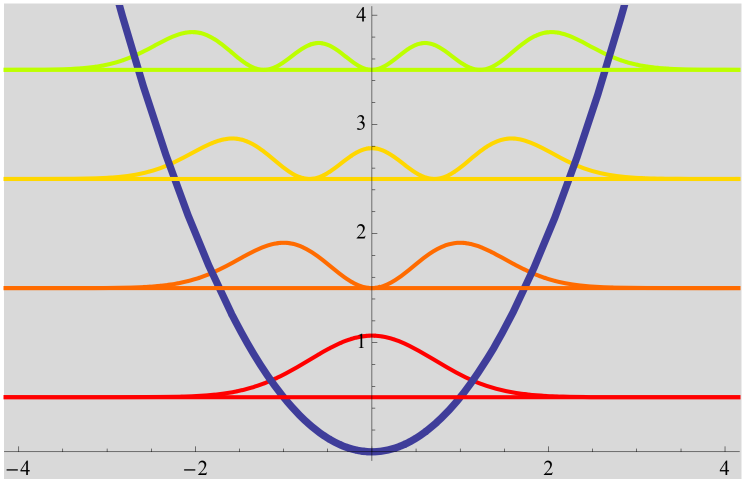


Fig.5

```
Show[plot1, plot2, plot3, PlotRange → {{-4, 4}, {0, 4}}]
```



Classical limit

`wc[ξ_, n_] :=`

$$\frac{1}{\pi\sqrt{2n+1}}\;\frac{1}{\sqrt{1-\frac{\xi^2}{2n+1}}}$$

```
dplot1 = Plot[Evaluate[wc[ξ, 30]], {ξ, -7, 7}, PlotStyle → {Thick, Blue},
   PlotRange → All, Background → LightGray];

dplot2 = Plot[Evaluate[φ[30, ξ]^2], {ξ, -10, 10}, PlotPoints → 100,
   PlotStyle → {Thick, Hue[0]}, PlotRange → All, Background → LightGray];

g1 = Graphics[{ Text[Style["Classical limit", Black, 15], {-5, 0.07}],
    Text[Style["n = 30", Black, 20], {1, 0.15}]}] ;

Show[dplot1, dplot2, g1]
```

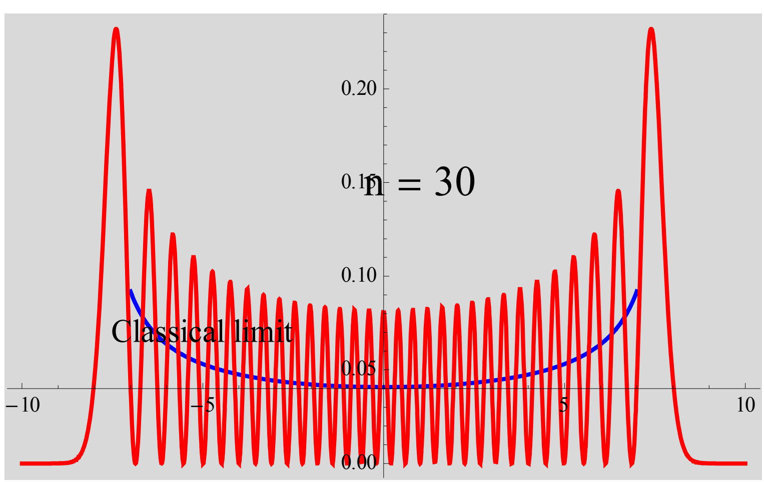


Fig.6 and 7

6.22 One dimensional Schrödinger equation

We consider the one dimensional motion of a particle in a potential energy $V(x)$. The Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+V(x)\psi(x)=E\psi(x),$$

or

$$\frac{d^2}{dx^2}\psi(x)-\frac{2m}{\hbar^2}V(x)\psi(x)+\frac{2m}{\hbar^2}E\psi(x)=0.$$

This equation is rewritten as

$$L\psi(x)+\lambda\psi(x)=0,$$

where

$$L\psi(x)=\frac{d^2}{dx^2}\psi(x)+q(x)\psi(x), \qquad \lambda=\frac{2m}{\hbar^2}E,$$

with

$$q(x)=-\frac{2m}{\hbar^2}V(x).$$

L is the self-adjoint operator, and λ is the eigenvalue. The weight function is $w(x) = 1$.

6.23 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 $2a$ 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.

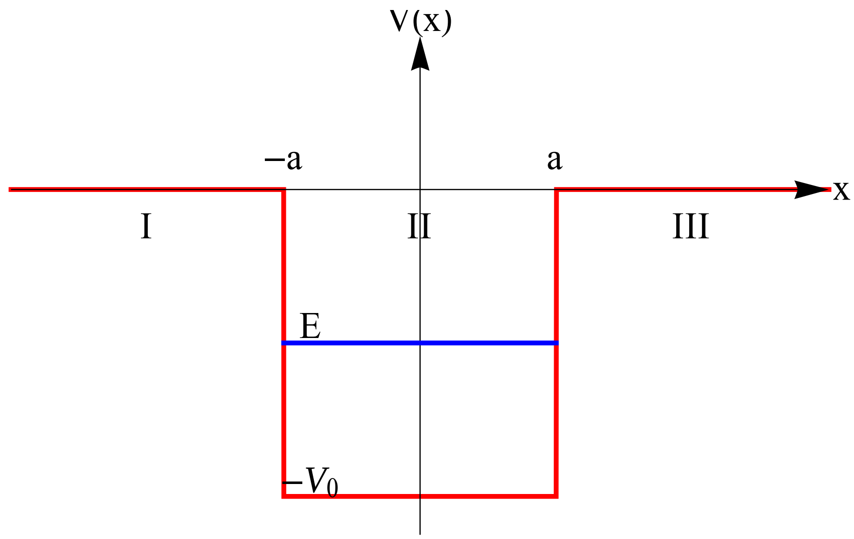


Fig.8 One dimensional square well potential of width 2a and depth V_0.

(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 $\frac{d\varphi(x)}{dx}$ 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 $\dfrac{d\varphi(x)}{dx}$ 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.

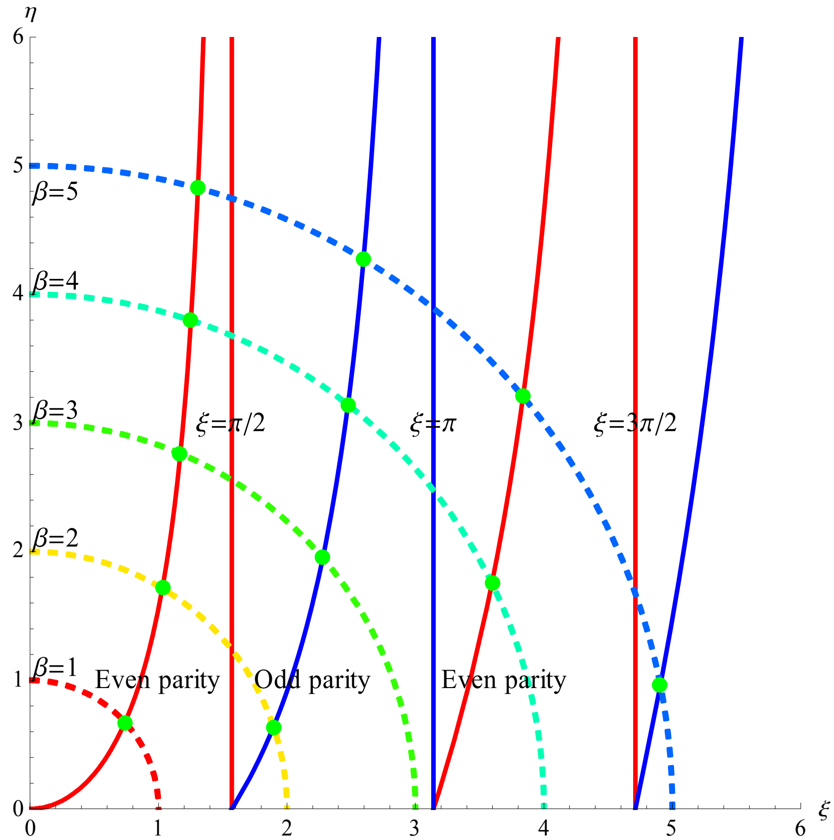


Fig.9 Graphical solution. One solution with even parity for $0<\beta<\pi/2$. One solution with even parity and one solution with odd parity for $\pi/2<\beta<\pi$. Two solutions with even parity and one solution with odd parity for $\pi<\beta<3\pi/2$. Two solutions with even parity and two solutions with odd parity for $3\pi/2<\beta<2\pi$. $\eta = \xi \tan\xi$ 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. $\varepsilon = \dfrac{|E|}{V_0} = \dfrac{\eta^2}{\beta^2} = 1-\dfrac{\xi^2}{\beta^2}$. $\xi = ka$ and $\eta = \kappa a$.

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

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

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

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

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

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

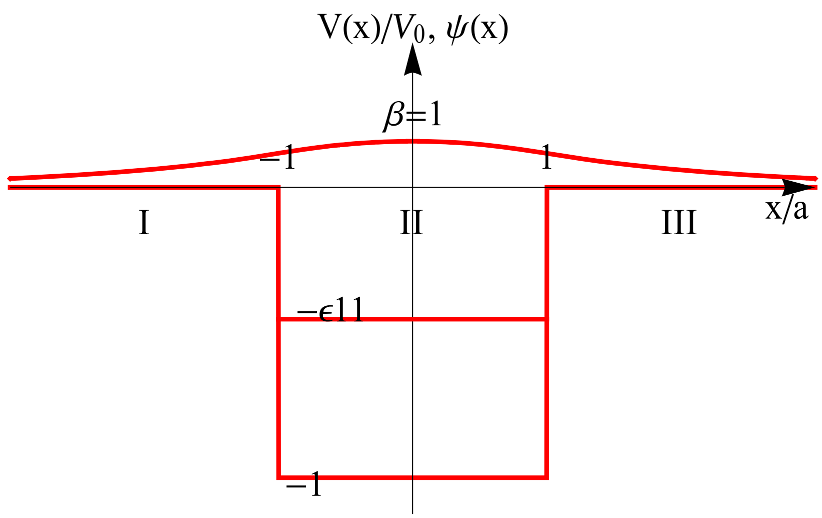

Fig.10 Square well potential $V(x)$ of width $2a$ and depth V_0. β = 1 and the corresponding wavefunction $\psi(x)$ which is normalized. There is one bound state (even parity) (- ε_{11} = -0.45735), where $\varepsilon = |E|/V_0$.

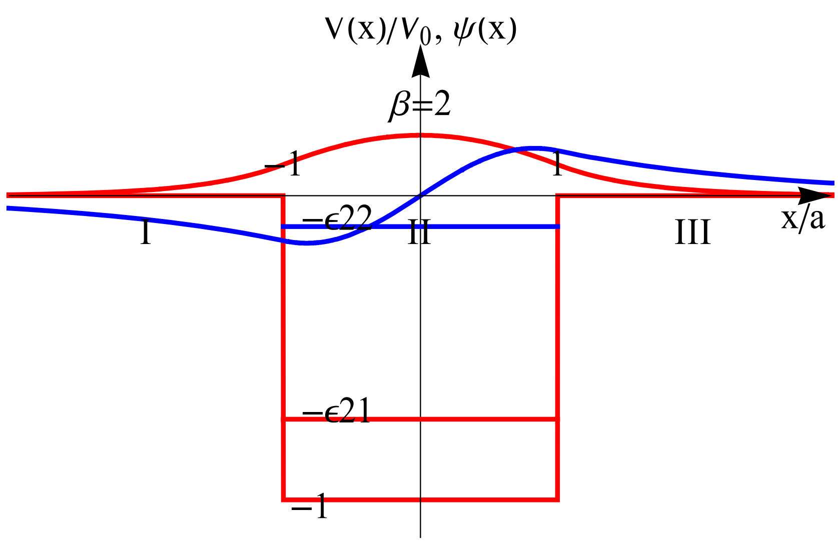

Fig.11 β = 2. There are two bound states. (i) The bound state (denoted by red) with even parity (- ε_{21} = -0.734844). (ii) The bound state (denoted by blue) with odd parity (-ε_{22} = -0.101775).

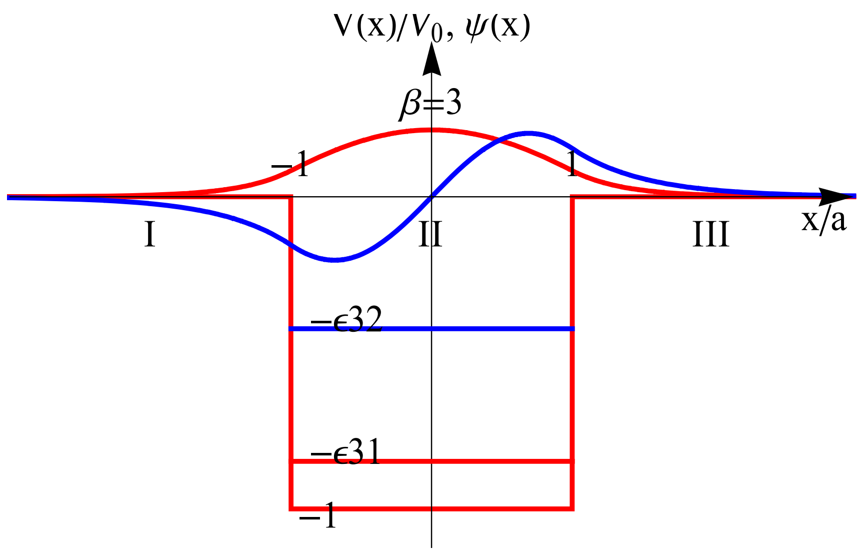

Fig.12 β = 3. There are two bound states. (i) The bound state (denoted by red) with even parity (-ε_{31} = -0.847869). (ii) The bound state (denoted by blue) with odd parity (-ε_{32} = -0.422976).

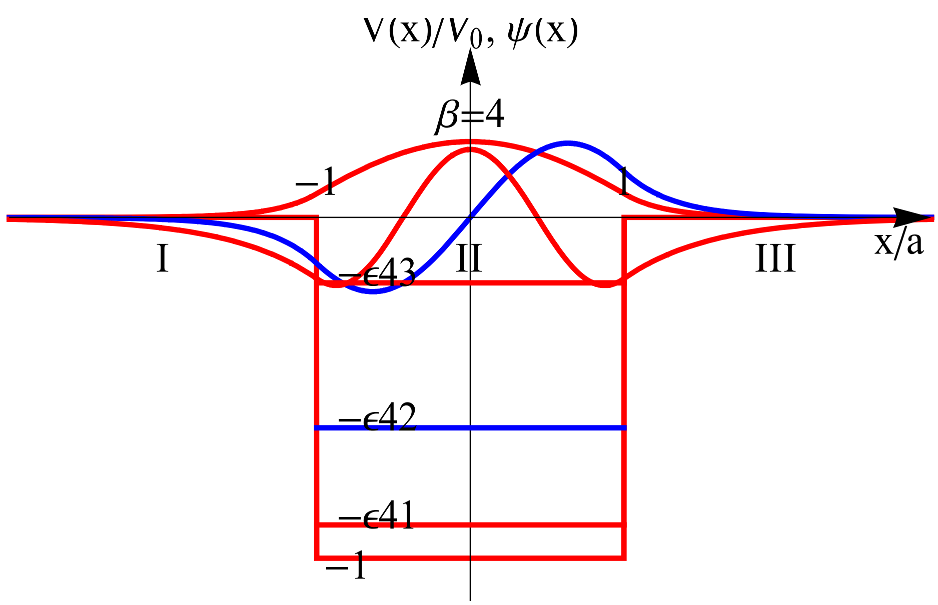

Fig.13 β = 4. There are three bound states. (i) The bound state (denoted by red) with even parity (-ε_{41} = -0.901976). (ii) The bound state (denoted by blue) with odd parity ($-\varepsilon_{42}$ = -0.617279). (iii) The bound state (denoted by red) with even parity ($-\varepsilon_{43}$ = -0.192111).

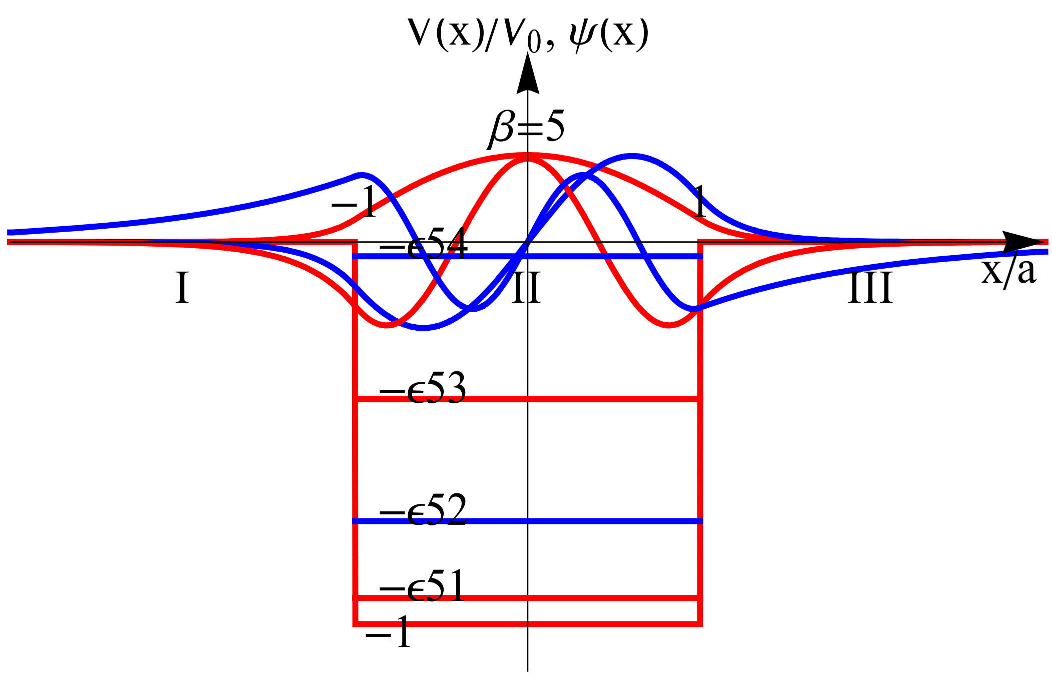

Fig.14 β = 5. There are four bound states. (i) The bound state (denoted by red) with even parity ($-\varepsilon_{51}$ = -0.931729). (ii) The bound state (denoted by blue) with odd parity ($-\varepsilon_{52}$ = -0.730486). (iii) The bound state (denoted by red) with even parity ($-\varepsilon_{53}$ =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

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