Lecture 6: Exactly Solvable One - Dimensional Problems

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1 Introduction: The Art and Craft of Solving Schroedinger Equation

Very few problems can be solved exactly in quantum mechanics. However they have important role in solving more general problems in which approximation methods are applied.

1.1 Method of Commuting Operators

To solving quantum mechanical problem in the case of stationary states, means to solve Schroedinger wave equation by obtaining the eigenstates and eigenvalues. There are several ways of accomplishing this task and one of the most practical approaches is the method of *commuting operators*. In this approach we identify operators that commute with the Hamiltonian of the system and depend on the same variables that Hamiltonian does. With this way, by applying the property that commuting operators have same eigenstates one can sometime guess the most appropriate form of the eigenstate of the Hamiltonian. Thus in this approach the task is to identify operators that commute with H and use these operators to obtain the eigenstates of the hamiltonian.

2 Quantum Systems with One Dimensional Potential

We first consider one dimensional quantum systems for which the general form of the Hamiltonian has the form:

$$H = \frac{1}{2m}p^2 + V(x).$$
 (1)

Since $[\hat{p}\hat{H}] \neq 0$ one expects no comment eigenstates for momentum and Hamiltonian operators. With the above Hamiltonian the Schroedinger equation for the bound state reads:

With the above Hamiltonian the Schroedinger equation for the bound state reads:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi_n(x) = E_n\psi_n(x).$$
(2)

With this equation one needs to obtain both the eigenfunctions, $\psi_n(x)$ and eigenvalues E_n and there are several approaches for the limited number of quantum systems for which one has exact analytic solutions.

One of the methods is the method of commuting operators which we will consider below.

3 Using symmetry properties of Hamiltonian to solve Schroedinger equations

One of the most powerful methods to identify operators that commute with Hamiltonian is to consider the symmetry properties of Hamiltonian. If such a symmetry is found that one expects that operator, \hat{A} characterizing the given symmetry will commute with \hat{H}

$$[\hat{A}\hat{H}] = 0 \tag{3}$$

Then one use the operator \hat{A} to find the eigenstate of \hat{H} .

3.1 Space inversion operator

In one-dimensional problems one of the most important property to consider is the symmetry of the quantum system with respect of the space inversion. To defined the operators of space inversion we recall the eigenstates of coordinate and momentum operators $| \psi_x \rangle$ and $| \phi_p \rangle$ for which the space translation operator, \mathcal{R} is defined as follows:

$$\mathcal{R} | \psi_{\pm x} \rangle = | \psi_{\mp x} \rangle \text{ and } \mathcal{R} | \phi_{\pm p} \rangle = | \phi_{\mp} \rangle.$$
 (4)

Using the normalization properties of coordinate and momentum eigenstates:

$$\langle \psi_{\pm x'} | \psi_{\pm x} \rangle = \delta(x - x') \text{ and } \langle \phi_{\pm p'} | \psi_{\pm p} \rangle = \delta(p - p')$$
 (5)

on obtains the unitarity condition for operators \mathcal{R} :

$$R^{\dagger}R = I. \tag{6}$$

Furthermore, from Eq.(4) one has:

$$\mathcal{R}^2 | \psi_{\pm x} \rangle = \mathcal{R} | \psi_{\mp x} \rangle = | \psi_{\pm x} \rangle \text{ and } \mathcal{R}^2 | \phi_{\pm p} \rangle = \mathcal{R} | \phi_{\mp p} \rangle = | \phi_{\pm p} \rangle$$
(7)

from which it follows:

$$\mathcal{R}^2 = I. \tag{8}$$

From Eq.(6) and (8) one observes that parity operator is an hermitian operator and equals to its inverse:

$$\mathcal{R}^{\dagger} = \mathcal{R} = \mathcal{R}^{-1} \tag{9}$$

Hermitivity of the operator indicates that the eigenvalues of the operator should be a real numbers. From Eq.(8) one then observes that the possible eigenvalues of operator \mathcal{R} are ± 1 . Thus one can identify to distinct eigenstates of operator $\mathcal{R} \psi_{\pm}$ satisfying the relation:

$$\mathcal{R} \mid \psi_{\pm} \rangle = \pm \mid \psi_{\pm} \rangle. \tag{10}$$

The $|\psi_{\pm}\rangle$ states usually referred to as positive and negative parity states.

It is useful also to show that the parity operator \mathcal{R} is not commuting with the coordinate and momentum operators however their anti-commutator is equal to zero:

$$[\hat{x}\hat{\mathcal{R}}] = 2\hat{x}\hat{\mathcal{R}} \quad \text{and} \quad \hat{x}\hat{\mathcal{R}} + \hat{\mathcal{R}}\hat{x} = 0 [\hat{p}\hat{\mathcal{R}}] = 2\hat{p}\hat{\mathcal{R}} \quad \text{and} \quad \hat{p}\hat{\mathcal{R}} + \hat{\mathcal{R}}\hat{p} = 0$$
(11)

3.2 Degeneracy Theorem

For further discussion it is useful to discuss the following property that indicates an existence for the degeneracy for the eigenvalues of Hamiltonian, when the different eigenstates have same energy eigenvalues.

3.3 One Dimensional Motion of Free Particle

For the case of free particle the Hamiltonian operator has the most simple form:

$$\hat{H} = \frac{\hat{p}^2}{2m}.\tag{12}$$

With Schroedinger wave equation in the form:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) = E\psi_n(x).$$
(13)

For such Hamiltonian from Eq.(4) it follows that:

$$[H\mathcal{R}] = 0,\tag{14}$$

thus the eigenstates of \mathcal{R} can be used to identify the eigenstates of \dot{H} . The wave function of eigenstates that satisfy Eq.(10) are $\psi_+(x) = A\cos(\frac{p}{\hbar}x)$ and $\psi_-(x) = -B\sin(\frac{p}{\hbar}x)$ corresponding to positive and negative parity states respectively for the particle with momentum magnitude p. Inserting both wave functions into Eq.(3.3) one obtains for both cases:

$$E_{\pm} = \frac{p^2}{2m}.\tag{15}$$

This example indicates that the energy of the free motion is degenerate in which case different parity states have same energy.

The same commutating operator method can be used to find different set of eigenstates of free Hamiltonian, noticing that

$$[\hat{H}\hat{p}] = 0. \tag{16}$$

In this case one can use the eigenfunctions of the momentum operator $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{-i\frac{p}{\hbar}x}$ and $\psi_{-p}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}$ which correspond to the one-dimensional motion with positive and negative momentum $\pm p$, as an eigenfunction for the Hamiltonian \hat{H} . Inserting these functions into Eq.() one obtains:

$$E(\pm p) = \frac{p^2}{2m},\tag{17}$$

which again indicates that the energy of the free motion is degenerate, but in this case for different direction of the motion of the quantum particle.

It is worth mentioning that while Eq.(14) indicates on the space reversal symmetry of the quantum system, Eq.(16) is an indication that the quantum system has a translational symmetry, that is it is symmetric with respect to the space translation in x direction.

4 One Dimensional Infinite Square Well

We now consider a quantum particle in the infinite potential well. Quantum mechanically the concept of infinite momentum well is defined such that probability of finding a particle at any point outside the well is strictly zero. In coordinate projection of the state vector of the particle will result to the following condition for the wave function of the particle:

$$\psi(x) = 0 \quad \text{for} \quad |x| > a \tag{18}$$

where a characterizes the size of one-dimensional well. It is customary the above condition to express through the condition on the potential energy as follows:

$$V(x) = \begin{cases} 0 & \text{if } |x| < a;\\ \infty & \text{if } |x| \ge a. \end{cases}$$
(19)

In this case the hamiltonian \hat{H}

$$\hat{H} = \frac{p^2}{2m} + V(x)$$
 (20)

has explicit symmetry with respect to the space reflection

$$[\hat{H}\hat{\mathcal{R}}] = 0 \tag{21}$$

thus one can chose of the eigenstates the \pm parity eigenstates. For the corresponding wave functions satisfying Schroedinger wave equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{n,\pm}(x)}{dx^2} + V(x)\psi_{n,\pm}(x) = E_n^{\pm}\psi_{n,\pm}(x).$$
(22)

one can choose:

$$\psi_{n,+}(x) = A\cos(k_+x)$$

$$\psi_{n,-}(x) = B\sin(k_-x)$$
(23)

which are clearly an eigenstates of \mathcal{H} at |x| < a as well as for space inversion operator \mathcal{R} . Inserting wave functions in Eq.(24) into Eq.(22) for |x| < a one obtains:

$$E_n^{\pm} = \frac{\hbar^2 k_{\pm}^2}{2m}.$$
 (24)

To estimate k_{\pm} we notice from condition of Eq.(18) that that

$$\psi_{\pm}(x) = 0, \text{ for all } x > a. \tag{25}$$

Then the requirement of the continuity of the wave function results in a condition:

$$\psi_{\pm}(a) = \psi_{\pm}(-a) = 0. \tag{26}$$

Using Eq.(24) for positive parity states one obtain:

$$A\cos(k_{+}a) = A\cos(-k_{+}a) = 0,$$
(27)

from which one obtains:

$$k_{+}a = n\frac{\pi}{2}, \quad k_{+} = n\frac{\pi}{2a} \quad \text{for odd} \quad n's.$$
 (28)

For negative parity states:

$$B\sin(k_{-}a) = A\sin(-k_{-}a) = 0,$$
(29)

from which one obtains:

$$k_{-}a = (n+1)\pi, \quad k_{-} = (2n+2)\frac{\pi}{2a} \quad \text{for all} \quad n's \quad \text{or} k_{-} = n\frac{\pi}{2a} \text{for even} \quad n's.$$
 (30)

Combining above two equations on can write

$$k_n^{pm} = \frac{\pi n}{2a} \tag{31}$$

where odd n's defined positive parity states momenta and even n's the same for the negative parity. At last one can defined normalization constants A and B from the condition

$$A^{2} \int_{-a}^{a} \cos^{2}(k_{+}x) dx = 1 \quad \text{and} \quad B^{2} \int_{-a}^{a} \sin^{2}(k_{-}x) dx = 1$$
(32)

resulting in $A = B = \frac{1}{\sqrt{a}}$). Thus the wave functions of the particle inside of the infinite momentum well are

$$\psi_n^+(x) = \frac{1}{\sqrt{a}}\cos(\frac{n\pi}{2a}x) \text{ with odd } n's$$

$$\psi_n^-(x) = \frac{1}{\sqrt{a}}\sin(\frac{n\pi}{2a}x) \text{ with even } n's.$$
(33)

Note that the lower possible value of n = 1 which will correspond to the ground sate and it is a positive parity state. The n=0 gives $\psi = 0$, a trivial solution that has no physical significance.

4.0.1 Expectations

It is instructive to evaluate expectation values of several observables, that in some sense defines the picture of quantum particle observed by "classical" observed.

First we estimate the expectation values of position \hat{x} and momentum \hat{p} operators:

$$\langle \hat{x} \rangle_{+} = \int_{-a}^{a} x |\psi_{n}^{+}(x)|^{2} dx = \frac{1}{a} \int_{-a}^{a} x \cos^{2} (k_{n}^{+}x) dx = \frac{1}{2a} \int_{-a}^{a} x (1 + \cos (2k_{n,+}x)) dx = 0$$

$$\langle \hat{x} \rangle_{-} = \int_{-a}^{a} x |\psi_{n}^{-}(x)|^{2} dx = \frac{1}{a} \int_{-a}^{a} x \sin^{2} (k_{n}^{+}x) dx = \frac{1}{2a} \int_{-a}^{a} x (1 - \cos (2k_{n,+}x)) dx = 0$$

$$(34)$$

$$\langle \hat{p} \rangle_{+} = \int_{-a}^{a} \psi_{n}^{+}(x)^{\dagger}(-i\hbar) \frac{d}{dx} \psi_{n}^{+}(x) dx = \frac{ik_{n}^{+}\hbar}{a} \int_{-a}^{a} \cos\left(k_{n}^{+}x\right) \sin\left(k_{n}^{+}x\right) dx = \frac{ik_{n}^{+}\hbar}{2a} \int_{-a}^{a} \sin(2k_{n}^{+}x) dx = 0$$

$$\langle \hat{p} \rangle_{-} = \int_{-a}^{a} \psi_{n}^{-}(x)^{\dagger}(-i\hbar) \frac{d}{dx} \psi_{n}^{-}(x) dx = \frac{-ik_{n}^{-}\hbar}{a} \int_{-a}^{a} \sin\left(k_{n}^{-}x\right) \cos\left(k_{n}^{-}x\right) dx = \frac{-ik_{n}^{-}\hbar}{2a} \int_{-a}^{a} \sin(2k_{n}^{-}x) dx = 0$$

$$(35)$$

$$\langle \hat{x}^2 \rangle_+ = \int_{-a}^{a} x^2 |\psi_n^+(x)|^2 dx = \frac{1}{a} \int_{-a}^{a} x^2 \cos^2(k_n^+ x) dx = a^2 \left(\frac{n^2 \pi^2 - 6}{3n^2 \pi^2}\right), \quad n \text{ odd}$$

$$\langle \hat{x}^2 \rangle_- = \int_{-a}^{a} x^2 |\psi_n^-(x)|^2 dx = \frac{1}{a} \int_{-a}^{a} x^2 \sin^2(k_n^+ x) dx = a^2 \left(\frac{n^2 \pi^2 - 6}{3n^2 \pi^2}\right), \quad n \text{ odd}$$

$$(36)$$

$$\langle \hat{p}^2 \rangle_+ = -\hbar^2 \int_{-a}^{a} \psi_n^+(x)^{\dagger} \frac{d^2}{dx^2} \psi_n^+(x) dx = \frac{(k_n^+)^2 \hbar^2}{a} \int_{-a}^{a} \cos^2(k_n^+ x) dx = (k_n^+)^2 \hbar^2 = \frac{n^2 \pi^2 \hbar^2}{4a^2}, \quad n \text{ odd}$$

$$\langle \hat{p}^2 \rangle_- = -\hbar^2 \int_{-a}^{a} \psi_n^-(x)^{\dagger} \frac{d^2}{dx^2} \psi_n^-(x) dx = \frac{(k_n^-)^2 \hbar^2}{a} \int_{-a}^{a} \sin^2(k_n^- x) dx = (k_n^-)^2 \hbar^2 = \frac{n^2 \pi^2 \hbar^2}{4a^2}, \quad n \text{ even}$$

$$(37)$$

4.1 Heisenberg Uncertainty in the Well

The above calculated expectations allow to check the Heisenberg uncertainty for the quantum particle in the infinite well. In this case

$$\sigma_x^2 = \langle | (\hat{x} - \langle x \rangle)^2 | \rangle^2 = \langle | \hat{x}^2 | \rangle \equiv x_{rms}^2 = a^2 \left(\frac{n^2 \pi^2 - 6}{3n^2 \pi^2} \right),$$
(38)
$$\sigma_p^2 = \langle | (\hat{p} - \langle p \rangle)^2 | \rangle^2 = \langle | \hat{p}^2 | \rangle \equiv p_{rms}^2 = \frac{n^2 \pi^2 \hbar^2}{4a^2},$$

from which it follows that

$$\sigma_x^2 \sigma_p^2 = \frac{\hbar^2}{4} \left(\frac{n^2}{3} - \frac{2}{\pi^2}\right) > \frac{\hbar^2}{4} \tag{39}$$

which shows that Heisenberg uncertainty is satisfied.

It is interesting to note that because $\langle x \rangle = \langle p \rangle$ the variances σ_x and σ_p are related to the RMS values of the measured coordinate and position of the quantum particle. As it follows from Eq.(37) the RMS values of the momentum grows linearly with n while the RMS value of the position x becomes localized at $x_{rms} \mid_{n \to \infty} = \frac{a}{3}$.

4.2 Discontinuities at the Border

As it was shown during the discussion of "seven wisdoms" of Schroedinger equation, the wave function's first derivative has a discontinuity for situation in which the potential energy operator contain an singularity (or is infinite). To calculate this discontinuity we estimate:

$$\Delta \psi'_{\pm}(a) \equiv \left(\psi'_{\pm}(a-\epsilon) - \psi'_{\pm}(a+\epsilon)\right)|_{\epsilon \to 0} \tag{40}$$

for which using relations from Eq.(34) one obtains:

$$\Delta \psi'_{+}(a) = -\frac{n\pi}{2a^{\frac{3}{2}}} \sin(\frac{n\pi}{2}) = \frac{n\pi}{2a^{\frac{3}{2}}} (-1)^{\frac{n+1}{2}}, n = \text{ odd},$$
(41)
$$\Delta \psi'_{-}(a) = \frac{n\pi}{2a^{\frac{3}{2}}} \cos(\frac{n\pi}{2}) = \frac{n\pi}{2a^{\frac{3}{2}}} (-1)^{\frac{n}{2}}, n = \text{ even}$$

5 One Dimensional Traps

Consider a potential energy:

$$V(x) = \begin{cases} -V_0 & \text{if } |x| < a; \\ 0 & \text{if } |x| \ge a. \end{cases}$$
(42)

with the Hamiltonian:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + V(x)$$
(43)

and looking for a Bound state solution. Since potential energy vanishes at infinity then the bound sates can happen only if E < 0. One observes that such a Hamiltonian do not commute with the momentum operator $[\hat{H}, \hat{p}] \neq = 0$. It is so because of the discontinuity of the potential at |x| = a. It however commutes with the space inversion operator $[\hat{H}, \hat{R}] = 0$ therefore one can look for the potential eigenstates of the Hamiltonian in the form of the eigenstates of \hat{R} operator.

To proceed we present the Schroedinger equation in three ranges according to Fig.??, for which one obtains:

I
$$\frac{\hbar^2}{2m} \nabla^2 \psi(x) = |E| \psi(x)$$

II
$$-\frac{\hbar^2}{2m} \nabla^2 \psi(x) = (V_0 - |E|)$$

III
$$\frac{\hbar^2}{2m} \nabla^2 \psi(x) = |E| \psi(x)$$
(44)

According to the wisdom number two energy of the bound state $E > V_{min}$ thus $|E| < V_0$. This relation allows to introduce $k = \sqrt{\frac{2m(V_0+E)}{\hbar^2}}$ for range II. For ranges I and III one introduces also $\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$.

As it follows from Eqs.(42) and (43) the Hamiltonian commutes with space translation operator \mathcal{R} therefore one expects that solutions should be also eigenstates of operator \mathcal{R} which mean with positive and negative eigenstates. Such solutions can be represented in the form: For positive eigenvalue of \mathcal{R} :

$$\psi_{+}(x) = Ae^{\kappa x}\Theta(-a-x) + Ae^{-\kappa x}\Theta(x-a) + C\cos kx \cdot \Theta(x+a)\Theta(a-x)$$
(45)

and for negative eigenvalue of \mathcal{R} :

$$\psi_{-}(x) = Be^{\kappa x}\Theta(-a-x) - Be^{-\kappa x}\Theta(x-a) + D\sin kx \cdot \Theta(x+a)\Theta(a-x)$$
(46)

Since the potential energy is finite everywhere one should expect that both the wave function and the first derivative should be continuous function: The continuity conditions should be considered at the boundary of the potential a or -a from which for the wave function and the derivative follows: for ψ_+ wave function:

$$Ae^{-\kappa a} = C\cos ka$$
$$-\kappa Ae^{-\kappa a} = -kC\sin ka \tag{47}$$

and for ψ_{-} wave function:

$$-Be^{-\kappa a} = D\sin ka$$

$$\kappa Be^{-\kappa a} = kD\cos ka$$
(48)

To continue with finding the eigenstates for both parity wave functions we divide the upper and lower parts of the above equations to obtain:

(+)
$$\kappa \cot ka = k$$

(-) $k \cot ka = -\kappa$ (49)

The above relations represent a transcendental equations and can be solved only numerically. To proceed let us make following definitions:

$$x = ka, \quad y_{+} = x \tan x, \quad y_{-} = x \cot x \quad \text{and} \quad R^{2} = \frac{2mV_{0}a^{2}}{\hbar^{2}}$$
 (50)

Then Eq.49 for "+" and "-" parities will have same expressions as

$$(+) y_{+} = \frac{x\kappa}{k}$$

$$(-) y_{-} = \frac{x\kappa}{k} (51)$$

One can now show that for both parities:

$$x^2 + y_{\pm}^2 = R^2 \tag{52}$$

where on the other hand:

(+)
$$x^{2} + y_{+}^{2} = \frac{x^{2}}{\cos x^{2}}$$

(-) $x^{2} + y_{-}^{2} = \frac{x^{2}}{\sin x^{2}}$ (53)

Comparing Eqs.(52) and (53) we obtain the simplified version of Eq.(49) which can be solved numerically:

$$(+) \qquad \frac{x}{\cos x} = R$$

$$(-) \qquad \frac{x}{\sin x} = R \qquad (54)$$

The solutions in this case correspond to the interception of $\frac{x}{\cos x}$ and $\frac{x}{\sin x}$ with constant R see Fig1. As the figure shows the lowest possible R will have solution only for the positive parity states while the negative parity requires a minimal value for R to have an intercepts.

The intercepts allow to obtain solutions for x = ka from which one obtains k. Once k is known the energy values can be calculate using the relation $k = \sqrt{\frac{2m(V_0+E)}{\hbar^2}}$, which results in $E = \frac{\hbar^2 k^2}{2m} - V_0$.



Figure 1: Red curves positive parity, blue curves negative parity solutions. Green lines are different values of R.

5.1 Low Momentum Narrow and Deep Trap Solution

We now consider the low momentum narrow and deep trap solution with the condition $ka \ll 1$ and $|E| \ll |V_0|$. In this case, $\cot ka \approx \frac{1}{ka}$ and for Eq.(49) one obtains:

$$(+) \qquad \frac{\kappa}{ka} = k \quad \to \quad \kappa = ak^2$$
$$(-) \qquad \frac{k}{ka} = -\kappa \quad \to \quad 1 = -\kappa a.$$
(55)

Since κ by definition is a positive quantity, one observes that "(-)" parity does not have a solution at this limit. For positive parity from the above relation and the definitions of κ and k one obtains:

$$E = -\frac{2mV_0^2 a^2}{\hbar^2}$$
(56)

6 Problem with the δ -function like potential

We now consider a possibility of the existence of the bound states for the system in which the potential energy has a form of the δ function:

$$V = -\alpha\delta(x) \tag{57}$$

In this case the Hamiltonian a has a form:

$$\hat{H} = \frac{\hat{p}_x^2}{2m} - \alpha \delta(x) \tag{58}$$

and it clearly symmetric with respect to space inversion. From which it follows that

$$[\hat{R}, \hat{H}] = 0.$$
 (59)

Therefore to solve the Schroedinger wave equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) - \alpha\delta(x) = E\psi(x), \tag{60}$$

considering E < 0 cases since we are interested in the bound states We will look for the positive and negative helicity wave functions $\psi_{\pm}(x)$ which are eigenstates of $\hat{\mathcal{R}}$ operator.

Since for x < 0 and x > 0 the potential energy in Eq.(74) vanishes and solution for E < 0 corresponds to the exponentially decreasing wave functions. Using this fact the "+" and "-" helicity wave function can be constructed as follows: for the positive eigenvalue of $\hat{\mathcal{R}}$:

$$\psi_{+}(x) = A[e^{\kappa x}\Theta(-x) + e^{-\kappa x}\Theta(x)]$$
(61)

and for the negative eigenvalue of $\hat{\mathcal{R}}$:

$$\psi_{-}(x) = B[e^{\kappa x}\Theta(-x) - e^{-\kappa x}\Theta(x)]$$
(62)

where in both cases the parameter κ is not known.

Positive Parity Solution: We consider now the "+" -helicty wave function in Eq.(61 for which one obtains:

$$\psi'_{+} = \kappa A[e^{\kappa x}\Theta(-x) - e^{-\kappa x}\Theta(x)] - Ae^{\kappa x}\delta(-x) + Ae^{-\kappa x}\delta(x) = \kappa A[e^{\kappa x}\Theta(-x) - e^{-\kappa x}\Theta(x)]$$
(63)

where we used the relation $\frac{d\Theta(x)}{dx} = \delta(x)$ and

$$-Ae^{\kappa x}\delta(-x) + Ae^{-\kappa x}\delta(x) = -\delta(x) + \delta(x) = 0$$
(64)

Using Eq.(63) and above definition of δ function for the second derivative one obtains:

$$\psi_{+}^{\prime\prime}(x) = \kappa^{2} A[e^{\kappa x} \Theta(-x) + e^{-\kappa x} \Theta(x)] + \kappa A[-e^{\kappa x} \delta(-x) - e^{-\kappa x} \delta(x)] = \kappa^{2} \psi_{+}(x) - 2\kappa A \delta(x)$$
(65)

Inserting above relation into Eq.(74) one obtains:

$$-\frac{\hbar^2 \kappa^2}{2m} \psi_+(x) + \frac{\hbar^2 2\kappa}{2m} A\delta(x) - \alpha\delta(x)A = E\psi_+(x), \tag{66}$$

To solve above equation we note that only finite values of E are physical. Therefore one can fix the value of κ by requiring that the $\delta(x)$ function should be cancelled. This requirement results in:

$$\frac{\hbar^2}{2m} 2\kappa A = \alpha A \quad \to \quad \alpha = \frac{\hbar^2}{m} \kappa \quad \to \boxed{\kappa = \frac{m\alpha}{\hbar^2}} \tag{67}$$

The remaining part of Eq.(74) allows to calculate the energy which results in:

$$E = -\frac{\hbar^2 \kappa^2}{2m} = \frac{\hbar^2}{2m} \frac{m^2 \alpha^2}{\hbar^4} = -\frac{m\alpha^2}{2\hbar^2}$$
(68)

To find the constant A we use the normalization condition

$$\int_{-\infty}^{\infty} |\psi_{+}(x)|^{2} dx = 1$$
(69)

which results in

$$A^{2}\left[\int_{-\infty}^{0} e^{2\kappa x} dx + \int_{0}^{\infty} e^{-2\kappa x} dx\right] = \frac{A^{2}}{\kappa} = 1 \quad \rightarrow \boxed{A = \sqrt{\kappa} = \frac{\sqrt{m\alpha}}{\hbar}}$$
(70)

Thus the positive parity wave function will have the final form:

$$\psi_{+}(x) = \frac{\sqrt{m\alpha}}{\hbar} \left[e^{\frac{m\alpha}{\hbar^{2}}x} \Theta(-x) + e^{-\frac{m\alpha}{\hbar^{2}}} \Theta(x) \right]$$
(71)

Negative Parity Solution: We consider now the wave function of Eq.(62) from which one obtains:

$$\psi'_{-} = \kappa B[e^{\kappa x}\Theta(-x) + e^{-\kappa x}\Theta(x)] - Be^{\kappa x}\delta(-x) - Be^{-\kappa x}\delta(x)$$
(72)

and

$$\psi_{-}''(x) = \kappa^2 B[e^{\kappa x}\Theta(-x) - e^{-\kappa x}\Theta(x)] + B[-e^{\kappa x}\frac{\delta\delta(-x)}{dx} - e^{-\kappa x}\frac{d\delta(x)}{dx}] = \kappa^2 \psi_{-}(x) + B\delta'(x) - B\delta'(x) = \kappa^2 \psi_{-}(x)$$
(73)

Inserting above relation into Eq.(74) one obtains:

$$-\frac{\hbar^2 \kappa^2}{2m} \psi_-(x) - \alpha \delta(x) \psi_-(x) = E \psi_-(x) \quad \rightarrow \quad E = -\frac{\hbar^2}{2m} \kappa^2 - \alpha \delta(x) \tag{74}$$

This shows that "-" - parity wave function results in a singular binding energy for the system which is not - physical.

7 Canonical Quantization

7.1 General

Assume that the given Hamiltonian has the following form

$$H = A(q)a^{+}a + B(q) \tag{75}$$

where A(q) (positive) and B(q) are some functions and a is an operator satisfying following commutative relation

$$[aa^+] = 1 \tag{76}$$

Our goal is to calculate the energy spectrum of such hamiltonian.

Suppose we know the eigenstate of the hamiltonian $|\psi_n\rangle$ for given eigenvalue of E_n , that is

$$H|\psi_n\rangle = E_n|\psi_n\rangle \tag{77}$$

Then we consider

$$a^+|\psi_n\rangle = |\phi\rangle \tag{78}$$

which is again a state vector in the Hilbert space.

Let us check whether $|\phi\rangle$ is a eigenstate of H too.

$$H|\phi\rangle = Ha^{+}|\psi_{n}\rangle = A(q)a^{+}aa^{+}|\psi_{n}\rangle + B(q)a^{+}|\psi_{n}\rangle$$
(79)

From Eq.(76) we can substitute $aa^+ = 1 + a^+a$ which yields:

$$Ha^{+}|\psi_{n}\rangle = A(q)a^{+}a^{+}a|\psi_{n}\rangle A(q)a^{+}|\psi_{n}\rangle + B(q)a^{+}|\psi_{n}\rangle = a^{+}(H|\psi_{n}\rangle + A(q)|\psi_{n}\rangle)(80)$$

$$= (E_{n} + A(q))a^{+}|\psi_{n}\rangle$$
(81)

which means that $|\phi\rangle = a^+ |\psi_n\rangle$ is an eigenstate of the hamiltonian H with the eigenvalue of $E_n + A(q)$.

The similar derivation shows also that $a|\psi_n >$ is an eigenstate of Hamiltonian H with eigenvalue of $E_n - A(q)$.

Because of this property a^+ and a is called step up and step down operators.

It is easy to generalize that

 $(a^+)^n |\Psi_m\rangle$ will be an eigenstate with the eigenvalue of $E_m + n \cdot A(q)$

$$H(a^{+})^{n}|\Psi_{m}\rangle = (E_{m} + n \cdot A(q))(a^{+})^{n}|\Psi_{m}\rangle$$
(82)

and same way $(a^{-})^{n}|\Psi_{m}\rangle$ will be an eigenstate with the eigenvalue of $E_{m} - n \cdot A(q)$ and same way

7.2 Ground State

In the Hilbert space

$$\langle \phi | \phi \rangle = \langle \psi_n | a^+ a | \psi_n \rangle \ge 0$$
 (83)

Using Eq.(75) one can substitute in the above equation

$$a^+a = \frac{H - B(q)}{A(q)} \tag{84}$$

which results

$$\langle \psi_n | \frac{H - B(q)}{A(q)} | \psi_n \rangle = \frac{E_n - B(q)}{A(q)} \ge 0.$$
(85)

Because of positiveness of A(q), from the above equation one obtains

$$E_n \ge B(q) \tag{86}$$

Therefore the system has a ground state.

Let us assume the $|\psi_0\rangle$ corresponds to the ground state. Then according to the above discussion

$$a\psi_0\rangle = 0\tag{87}$$

since no state exists with lower energy. Multiplying above equation from the right by a^+ and using Eq.(75) one obtains

$$a^{+}a|\psi_{0}\rangle = \left(\frac{H - B(q)}{A(q)}\right)|\psi_{0}\rangle = \left(\frac{E_{0} - B(q)}{A(q)}\right)|\psi_{0}\rangle = 0$$
(88)

Again using the positiveness of A(q) one obtains

$$E_0 = B(q) \tag{89}$$

This together with Eq.(82) allows to obtain the energy spectrum of the system as

$$E_n = B(q) + nA(q) \tag{90}$$

It can be shown also that the normalized state vector for the n'th level can be expressed as:

$$|\psi_n\rangle = \frac{1}{\sqrt{n!}} (a^+)^n |\psi_0\rangle \tag{91}$$

7.3 Level Number Operator

One can introduce an operator $\hat{N} = a^+ a$ and demonstrate that

$$\hat{N}|\psi_n\rangle = \left(\frac{H - B(q)}{A(q)}\right)|\psi_n\rangle = \left(\frac{E_n - B(q)}{A(q)}\right)|\psi_n\rangle = n|\psi_n\rangle \tag{92}$$

It can be shown that

$$\left[\hat{N},\hat{H}\right] = 0. \tag{93}$$

Thus the eigenstates of \hat{N} are conserved quantities.

7.4 Matrix Elements

Since $a^+|\psi_n\rangle$ corresponds to the eigenstate with n+1 level energy, one can write

$$a^+|\psi_n\rangle = c_n|\psi_{n+1}\rangle \tag{94}$$

From the above equation we obtain

$$|c_n|^2 = \langle \psi_n | aa^+ | \psi_n \rangle = n+1 \tag{95}$$

where in the last step we used the cammutator of $[aa^+]$ and the definition of the level number operator. If we assume that c_n numbers are real we obtain

$$c_n = \sqrt{n+1} \tag{96}$$

and

$$a^{+}|\psi_{n}\rangle = \sqrt{n+1}|\psi_{n+1}\rangle \tag{97}$$

This relation allows to calculate the matrix elements of the operators a and a^+ in the form

$$a_{mn}^{+} = \sqrt{n+1}\delta_{m,n+1}$$

$$a_{mn} = \sqrt{n}\delta_{m,n-1}$$
(98)

8 One Dimensional Harmonic Oscillator

Starting with classical Hamiltonian function for Harmonic Oscillator:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2,$$
(99)

where k is the Force constant and $\omega = \sqrt{\frac{k}{m}}$ one constructs a quantum mechanical Hamiltonian operator in the following form:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2 \tag{100}$$

Introduce

$$\hat{P} = \frac{\hat{p}}{\sqrt{m}}$$
 and $\hat{Q} = \sqrt{m}\hat{x}$ (101)

Using these definitions one obtains:

$$[\hat{P}, \hat{Q}] = [\hat{p}, \hat{x}] = -i\hbar$$
 (102)

With these definitions the Hamiltonian in Eq.(100) simplifies to:

$$\hat{H} = \frac{1}{2} \left(\hat{P}^2 + \omega^2 \hat{Q}^2 \right) \tag{103}$$

8.1 Rising and Lowering Operators

Introduce:

$$\hat{a} = \frac{1}{\sqrt{2\omega\hbar}} (\omega \hat{Q} + i\hat{P}) \tag{104}$$

and

$$\hat{a}^{\dagger} = \frac{1}{\sqrt{2\omega\hbar}} (\omega \hat{Q} - i\hat{P}) \tag{105}$$

Clearly these operators are not hermitean since $\hat{a}^{\dagger} \neq \hat{a}$. Moreover using Eq.(102) one obtains:

$$[\hat{a}, \hat{a}^{\dagger}] = 1$$
 (106)

same as in Eq.(76).

Expressing now operators of \hat{Q} and \hat{P} through \hat{a}^{\dagger} and \hat{a} :

$$\hat{Q} = (\hat{a} + \hat{a}^{\dagger})\sqrt{\frac{\hbar}{2\omega}}$$
 and $\hat{P} = (\hat{a} - \hat{a}^{\dagger})\sqrt{\frac{\omega\hbar}{2}\frac{1}{i}}$ (107)

for the Hamiltonian operator of Eq.(103) one obtains:

$$\hat{H} = \hbar\omega(\hat{a}^{\dagger}a + \frac{1}{2}) \tag{108}$$

It is also useful to check that:

$$[\hat{a}, \hat{a}^{\dagger}a] = [\hat{a}, \hat{a}^{\dagger}]a + \hat{a}^{\dagger}[\hat{a}, \hat{a}] = \hat{a}$$
(109)

$$\begin{bmatrix} \hat{a}, \hat{H} \end{bmatrix} = \hbar \omega \hat{a} \begin{bmatrix} \hat{a}^{\dagger}, \hat{H} \end{bmatrix} = [\hat{H}, \hat{a}]^{\dagger} = -\hbar \omega \hat{a}^{\dagger}$$
(110)

With Eqs. $(108 \text{ and } (106) \text{ we recognize that the problem is similar to one we discussed in canonical quantization with Eqs. <math>(75)$ and (76) with

$$A(q) = \hbar \omega \quad \text{and} \quad B(q) = \frac{1}{2}\hbar \omega$$
 (111)

Thus we conclude that operators defined in Eqs.(104) and (105) represent the lowering and rising operators for the eigenstate of Harmonic Oscillator hamiltonian satisfying relation:

$$\ddot{H} \mid \psi_n \rangle = E_n \mid \psi_n \rangle. \tag{112}$$

8.2 Energy Spectrum

The energy spectrum of Harmonic Oscillator can be calculated using definitions from Sec.7.1 from which it follows:

$$E_n = B(q) + nA(q) = \hbar\omega(n + \frac{1}{2}), \qquad (113)$$

with the ground state energy being:

$$E_0 = \frac{\hbar\omega}{2}.\tag{114}$$

This result is very strange since it indicates that quantum Harmonic Oscillator has a null state energy, which means that any stable quantum state will have null energy which can sum up to infinity.

8.3 Ambiguity of the Ground State

The apparent solution of the null energy problem is ambiguity in choosing quantum Hamiltonian operator for Harmonic Oscillator. We discussed previously that we don't a priori know how the original quantum Hamiltonian looks and as a rule we construct it from classical hamiltonians. Such was the approach in constructing the Hamiltonian operator in Eq.(100). However we could also construct a quantum mechanical Hamiltonian that has arbitrary term proportional to $[\hat{x}, \hat{p}]$ that will yield same classical Hamiltonian in the form of Eq.(99) since in classical limit $[\hat{x}, \hat{p}] \to 0$.

For example the following Hamiltonian operator is as legitimate as the one in Eq.(100):

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x} + i\frac{\omega}{2}[\hat{x}, \hat{p}].$$
(115)

Using now the definitions of Sec.8.1 one obtain

$$\hat{H} = \hbar \omega \hat{a} \hat{a}^{\dagger} \tag{116}$$

for which the energy spectrum will be in the form pf

$$E_n = n\hbar\omega \tag{117}$$

with

$$E_0 = 0 \tag{118}$$

Thus the standard solution for quantum Harmonic Oscillator is to discard the null energy by shifting energy spectrum up by $\frac{\hbar\omega}{2}$ and calculate according to Eq.(117).

However there is some controversy whether one needs to ignore the null modes especially in the relativistic case.

8.4 Expectation Values of Quantum Harmonic Oscillator

The quantum eigenstates of HO represent the solution of equation:

$$\hat{H} \mid \psi_n \rangle = \left[\frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2 \right] \mid \psi_n \rangle = E_n \mid \psi_n \rangle, \tag{119}$$

with

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right) \tag{120}$$

At this stage it is useful to calculate the expectation values for kinematic, $\hat{T} = \frac{\hat{p}^2}{2m}$, and potential energies of HO $\hat{V}(x) = \frac{1}{2}m\omega^2 \hat{x}^2$.

For expectation value of kinetic energy one obtains:

$$\langle \psi_n \mid \hat{T} \mid \psi_n \rangle = \langle \psi_n \mid \frac{\hat{p}^2}{2m} \mid \psi_n \rangle = \frac{1}{2} \langle \psi_n \mid \hat{P}^2 \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a} - \hat{a}^{\dagger})^2 \mid \psi_n \rangle \frac{\omega\hbar}{4}, \tag{121}$$

where we used first the definition of Eq.(101) then relation for \hat{P} according to Eq.(107) We now elaborate the term:

$$\langle \psi_n \mid (\hat{a} - \hat{a}^{\dagger})^2 \mid \psi_n \rangle = \langle \psi_n \mid (\hat{a}\hat{a} + \hat{a}^{\dagger}\hat{a}^{\dagger} - \hat{a}\hat{a}^{\dagger} - \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{a} \mid \psi_n \rangle = -\langle \psi_n \mid (\hat{a}\hat{$$

where in the derivation above we used the facts that $\langle \psi_n \mid (\hat{a}\hat{a}) \mid \psi_n \rangle = \langle \psi_n \mid (\hat{a}^{\dagger}\hat{a}^{\dagger}) \mid \psi_n \rangle = 0$ and $[\hat{a}, \hat{a}^{\dagger}] = 1$.

Substituting now Eq.(122) into Eq.(121) and using definition of the Hamiltonian operator in Eq.(108) one obtains:

$$\langle \psi_n \mid \hat{T} \mid \psi_n \rangle = \langle \psi_n \mid \frac{\hat{p}^2}{2m} \mid \psi_n \rangle = \frac{1}{2} \langle \psi_n \mid \hat{P}^2 \mid \psi_n \rangle = \frac{\hbar\omega}{2} \langle \psi_n \mid \hat{a}^{\dagger}\hat{a} + \frac{1}{2} \mid \psi_n \rangle = \frac{1}{2} \langle \psi_n \mid \hat{H} \mid \psi_n \rangle = \frac{E_n}{2} (123)$$

With the similar approach one can calculate the expectation value of potential energy:

$$\langle \psi_n \mid \hat{V}(x) \mid \psi_n \rangle = \langle \psi_n \mid \frac{1}{2} m \omega^2 \hat{x}^2 \mid \psi_n \rangle = \frac{1}{2} \omega^2 \langle \psi_n \mid \hat{Q}^2 \mid \psi_n \rangle = \frac{\hbar \omega}{4} \langle \psi_n \mid (\hat{a} + \hat{a}^{\dagger})^2 \mid \psi_n \rangle, \quad (124)$$

where in the derivation we used the relations of Eq.(101) and definition of Eq.(107). Now similar to Eq.(122):

$$\langle \psi_n \mid (\hat{a} + \hat{a}^{\dagger})^2 \mid \psi_n \rangle = \langle \psi_n \mid (\hat{a}\hat{a} + \hat{a}^{\dagger}\hat{a}^{\dagger} + \hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = \langle \psi_n \mid (\hat{a}\hat{a}^{\dagger} + \hat{a}^{\dagger}\hat{a} \mid \psi_n \rangle = \langle \psi_n \mid (2\hat{a}^{\dagger}\hat{a} + 1) \mid \psi_n \rangle$$

$$(125)$$

Substituting this into Eq.(124) and using the expression for the Hamiltonian operator in Eq.(108) one obtains:

$$\langle \psi_n \mid \hat{V}(x) \mid \psi_n \rangle = \frac{\hbar\omega}{2} \langle \psi_n \mid \hat{a}^{\dagger} \hat{a} + \frac{1}{2} \mid \psi_n \rangle = \frac{1}{2} \langle \psi_n \mid \hat{H} \mid \psi_n \rangle = \frac{E_n}{2}$$
(126)

From Eqs.(123) and (126) one concludes that for the case of Harmonic Oscillator the expectation values of kinetic and potential energies, equally share the energy eigenvalue E_n of the Hamiltonian.

It will be nice two show the same result applying Virial Theorem to Harminic Oscillator

8.5 Wave Functions of Quantum Harmonic Oscillator

We now will try to obtain the wave function of Harmonic Oscillator in coordinate representation. In general we have to solve the Schroedinger equation for the wave functions in the form:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right]\psi_n(x) = E_n\psi_n(x)$$
(127)

which is second order differential equation.

However we can also solve this problem using the method of commuting operators we used earlier to obtain the eigenstates of hamiltonian. For this, from Eq.(??) we notice that for the ground state:

$$[\hat{a}\hat{H}] \mid \psi_0 \rangle = \hbar \omega \hat{a} \mid \psi_0 \rangle = 0 \tag{128}$$

The last part of the equation follows from the fact that \hat{a} is a lowering operator and it can not lower the ground state any more. Thus to obtain the wave function of the ground state we can solve

$$\langle \psi_x \mid \hat{a} \mid \psi_o \rangle = \langle \psi_x \mid \frac{1}{\sqrt{2\omega\hbar}} \left(\omega \hat{Q} + i \hat{P} \right) \mid \psi_0 \rangle = \frac{1}{\sqrt{2\omega\hbar}} \langle \psi_x \mid \left(\omega \sqrt{m} \hat{x} + \frac{i}{\sqrt{m}} \hat{p} \right) \mid \psi_0 \rangle =$$
(129)
$$\frac{1}{\sqrt{2\omega m\hbar}} \left(\omega m x + \hbar \frac{d}{dx} \right) \psi_0(x) = 0,$$

where in the above derivation we used definition of \hat{a} from Sec.8.1.

With above equation we arrived at first order differential equation:

$$\left(\omega mx + \hbar \frac{d}{dx}\right)\psi_0(x) = 0, \qquad (130)$$

which is simpler than Eq.(127). It can be solved by separating differentials:

$$-\frac{m\omega}{\hbar}xdx = \frac{d\psi_o}{\psi_0} \tag{131}$$

with the solution $\psi_0(x) = Ce^{-\frac{m\omega}{2\hbar}x^2}$, where C one can calculation from normalization condition

$$|C|^2 \int_{-\infty}^{+\infty} e^{-\frac{m\omega}{2\hbar}x^2} dx = 1, \qquad (132)$$

resulting in $C = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}}$. Thus for the ground state wave function one obtains:

$$\psi_0(x) = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$$
(133)

Wave functions of the excited states can be calculated using the relation of Eq.91 in the form

$$\psi_n(x) = \frac{1}{\sqrt{n!}} \langle \psi_x \mid (a^{\dagger})^n \mid \psi_0 \rangle.$$
(134)

For example for the first excited state:

$$\psi_1(x) = \langle \psi_x \mid a^{\dagger} \mid \psi_0 \rangle \tag{135}$$

and using relation of Eq.(105) one obtains:

$$\psi_1(x) = \frac{1}{\sqrt{2m\omega\hbar}} \left(m\omega x - \frac{d}{dx} \right) \psi_0(x) = \frac{1}{\sqrt{2m\omega\hbar}} \left(m\omega x\psi_0(x) - \hbar \frac{d}{dx}\psi_0(x) \right) =$$
(136)
$$= \sqrt{\frac{2m\omega}{\hbar}} \left[\frac{m\omega}{\pi\hbar} \right]^{\frac{1}{4}} x e^{-\frac{m\omega}{2\hbar}x^2}.$$

We can continue in this manner to calculate wave functions of other excited states. However one can obtain a compact formula for any excited state, if we introduce a variable:

$$z = x \sqrt{\frac{m\omega}{\hbar}} \tag{137}$$

for the first part of Eq.(137) one obtains

$$\psi_1(x) = \sqrt{\frac{1}{2m\omega\hbar}} \left(\frac{m\omega}{\sqrt{\frac{m\omega}{\hbar}}} z - \hbar \frac{d}{dz} \sqrt{\frac{m\omega}{\hbar}} \right) \left[\frac{m\omega}{\pi\hbar} \right]^{\frac{1}{4}} e^{-\frac{z^2}{2}} =$$

$$= \frac{1}{\sqrt{2}} \left[\frac{m\omega}{\pi\hbar} \right]^{\frac{1}{4}} \left(z - \frac{d}{dz} \right) e^{-\frac{z^2}{2}}.$$
(138)

With the same procedure we can show that

$$\psi_2(x) = \frac{1}{\sqrt{2^2 2!}} \left[\frac{m\omega}{\pi\hbar} \right]^{\frac{1}{4}} \left(z - \frac{d}{dz} \right)^2 e^{-\frac{z^2}{2}}$$
(139)

and for given n:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} \left(z - \frac{d}{dz}\right)^n e^{-\frac{z^2}{2}}.$$
(140)

One can work out the above equation into the form of Hermite Polynomials defined in the form:

$$H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n} e^{-z^2}.$$
(141)

For this we notice that

$$\left(z - \frac{d}{dz}\right)^n e^{-\frac{z^2}{2}} = (-1)^n e^{\frac{z^2}{2}} \frac{d^n}{dz^n} e^{-z^2}.$$
(142)

and substituting the above equation into Eq.(140) one obtains:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left[\frac{m\omega}{\pi\hbar} \right]^{\frac{1}{4}} (-1)^n e^{\frac{z^2}{2}} \frac{d^n}{dz^n} e^{-z^2} = \frac{1}{\sqrt{2^n n!}} \left[\frac{m\omega}{\pi\hbar} \right]^{\frac{1}{4}} e^{-\frac{z^2}{2}} H_n(z).$$
(143)