A Project on solving Time Independent Schrödinger Equation

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Abstract

The present project mainly deals with non relativistic schrodinger equation for different time independent potentials.It explores power series method for solving differential equations associated with particles' dynamics.Moreover,the project gives a brief introduction to relativistic realm of quantum mechanics,discussing the Klein Gordon Model and Dirac model.Free particle in a space with curled up dimension and implication of it being in a curled up dimension has also been studied.

KEYWORDS:

Time Independent Schrödinger equation,Particle in a Box,Simple & Truncated Harmonic Oscillator,Hydrogen Atom,Klein-Gordon Equation,Dirac Equation,Kaluza-Klein tower of particles,Extra dimension(curled up).

Introduction:

Quantum mechanics as we know today is a vast area of research and knowledge.The journey began in the year 1901,founded by Plank.Thereafter came Schrödinger,Dirac,Heisenberg,Bohr and so on.They all established the foundation stone of quantum mechanics.In this project the Schrödinger viewpoint of qm is taken.Several time independent potentials are taken and corresponding differential equations are solved and interpreted physically.The time independence leads to seperation of variable with seperation constant E,which later comes out to be the eigenvalue of hamiltonian.The states corrosponding a particular energy E is termed as stationary state.Later relativity is incorporated in qm to yield Klein Gordon & Dirac model.As an amazing outcome of this incorporation is prediction of spin and antiparticle.

1 Particle in one dimensional box:

let a particle be confined within a one dimensional box of length l,free of any force.We are free to choose potential as 0 inside the box,while outside the box,it is taken to be infinity for necessary confinement.

To summarize,
$V(x) = 0$ for $0 < x < l$;
$V(x) = \infty$ otherwise

Let $\psi(x)$ represents particle's state(spatial part).Then $\psi(x)$ evolves according to schrödinger equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi \tag{1}$$

where m is mass of the particle and E is energy of the particle

Solution:

Equation(1) can be written as follows:

$$\frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi \tag{2}$$

[As particle is confined,it is in bound state,clearly ,E is less than $V(\pm\infty)$]

$$= -k^2\psi$$

where $k = \frac{\sqrt{2mE}}{\hbar}$
So the solution is:

$$\psi(x) = A\exp(ikx) + B\exp(-ikx) \ for \ 0 < x < l$$

$$\psi(x) = 0 \ otherwise \ i.e. \ for \ x \geq l \ \& \ x \leq 0$$

Now $\psi(x)$ is known to be continuous.

$$\psi(0) = 0 \tag{3}$$

$$\psi(l) = 0 \tag{4}$$

Equation (3) yields:$A + B = 0$

$$\psi(x) = A(\exp(ikx) - \exp(-ikx)) \tag{5}$$

$$= 2Ai\sin(kl) \tag{6}$$

equation(4) & (6) yield: $2Ai\sin(kl) = 0$, implying $kl = n\pi$ which in turn implies $k^2 = \frac{n^2\pi^2}{l^2}$

$$\Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2ml^2} \tag{7}$$

$$\Rightarrow E_{n+1} - E_n = \frac{(2n+1)\pi^2\hbar^2}{2ml^2} \tag{8}$$

As m,l goes on increasing,the discreteness in energy vanishes and $E_{n+1} \rightarrow E_n$.Quantum mechanics becomes apparent when m,l is small enough as compared to$\hbar$t to validate the discreteness in energy.In our universe the value of $\hbar$ is small($\simeq 10^{-34}$).So quantum mechanics operates in small scale of the order 10^{-16}.For example,consider an electron trapped in such a box.Take $l = 10^{-16}m$ and energy gap to be 10^{-3}.The example illustrates had $\hbar$ having a greater value,quantum mechaanics operates in large scale too.This is known as correspondence principle.

We have not normalised (6) yet,

$$\int_0^l |\psi(x)|^2 dx = 1$$

$$\Rightarrow 4|A|^2 \int_0^l sin\frac{n\pi}{l}x = 1$$

$$\Rightarrow 2A = \sqrt{\frac{2}{l}}\exp(i\alpha)$$

$$\psi(x) = \sqrt{\frac{2}{l}}\exp(i\beta)\sin(\frac{n\pi}{l}x) \tag{9}$$

where $\beta = \alpha + \frac{\pi}{2}$

Hence the normalised wave function is :

$$\psi(x,t) = \sqrt{\frac{2}{l}}\sin(\frac{n\pi}{l}x)\exp(-\frac{in^2\pi^2\hbar}{2ml^2}t) \tag{10}$$

We drop the $\exp(i\beta)$term because it carries no physical significance when we take $\psi\psi^*$,it gets out of the integral by getting multiplied by $\exp(i\beta)$.

2 Potential Barrier:

Let a particle with energy E incident from $-\infty$.It confronts potential barrier of V_0.We have 3 regions:

- Region 1:$-\infty < x < 0, \ V = 0$

- Region 2: $0 \leq x \leq l,\ V = V_0$
- Region 3: $x > l,\ V = 0$

Now we will study 3 cases:

- $E > V_0$
- $E = V_0$
- $E < V_0$

The corresponding Schrődinger equation for describing region 1 & 3 is:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi \tag{11}$$

Solution:

$$\psi_1(x) = A\exp(\imath kx) + B\exp(-\imath k_0 x) \tag{12}$$

$$\psi_3(x) = F\exp(\imath k_0 x) + G\exp(-\imath k_0 x) \tag{13}$$

where $k_0 = \frac{\sqrt{2mE}}{\hbar}$

We interpret $\exp(\imath k_0 x)$ as a wave travelling to the right while $\exp(-\imath k_0 x)$ represents wave travelling to the left.As the particles are coming from left i.e $-\infty$,the physical situation demands $G = 0$.

$$\psi_3(x) = F\exp(\imath k_0 x) \tag{14}$$

- Case 1:$E > V_0$

The corresponding schrődinger equation to describe region 2 is:

$$\frac{d^2\psi}{dx^2} = \frac{-2m(E - V_0)}{\hbar^2}\psi \tag{15}$$

$$\Rightarrow \psi_2(x) = C\exp(\imath kx) + D\exp(-\imath kx) \tag{16}$$

where $k = \frac{\sqrt{2m(E-V_0)}}{\hbar}$

The continuity of $\psi(x)$ & $\frac{d\psi(x)}{dx}$ at $x = 0$ & l and following elimination of C and D yield:

$$\frac{F}{A} = \frac{2k_0 k\exp[\imath l(k - k_0)]}{(k + k_0)^2 - (k_0 - k)^2\exp(2\imath kl)} \tag{17}$$

$$\frac{B}{A} = \frac{(k_0^2 - k^2)(1 - \exp(2\imath kl))}{(k + k_0)^2 - (k_0 - k)^2\exp(2\imath kl)} \tag{18}$$

$$T = |\frac{F}{A}|^2 = \frac{16k^2k_0^2}{(k + k_0)^4 + (k_0 - k)^4 - 2(k_0^2 - k^2)\cos(2kl)} \tag{19}$$

$$R = |\frac{B}{A}|^2 = \frac{2(k_0^2 - k^2)(1 - \cos(2kl))}{(k + k_0)^4 + (k_0 - k)^4 - 2(k_0^2 - k^2)\cos(2kl)} \tag{20}$$

If we add R to T,we get 1,rather astonoshing result.

Physical interpretation of R and T:

$A\exp(\imath k_0 x)$ represents wave travelling to the right, $B\exp(-\imath k_0 x)$ can be interpreted as reflected wave & $F\exp(\imath k_0 x)$ represents transmitted wave.Since,amplitude squared gives us intensity,we interpret R & T as probability of particle being reflected and transmitted respectively.$R + T = 1$confirms the particle is either reflected or transmitted to region 3.Classically,for $E > V_0$,the particle will always go to region 3.But quantum mechanically,there is a finite probability that the particle will be reflected back to region 1.In case,$V_0 = 0$ i.e. there is no barrier,R becomes 0 as$k_0 = k$.Physically,this is true too.As there is no barrier,the particle will always go through to region 3.

- Case 2:$E = V_0$

$$\frac{d^2\psi}{dx^2} = 0$$

$$\psi_2(x) = C + Dx \tag{21}$$

Elimination of C & D and continuity condition leads to:

$$R = \frac{k_0^2 l^2}{4 + k_0^2 l^2} \tag{22}$$

$$T = \frac{4}{4 + k_0^2 l^2} \tag{23}$$

Here also,$R + T = 1$.There is a finite probability of particle being reflected back even though clasically it should not be.

- Case 3:$E < V_0$

$$\frac{d^2\psi}{dx^2} = \frac{-2m(E - V_0)}{\hbar^2}\psi \tag{24}$$

$$= k^2\psi$$

where $k = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

$$\psi_2(x) = C\exp(kx) + D\exp(-kx) \tag{25}$$

Eliminating C & D we get:

$$T = \frac{16k_0^2k^2\exp(2kl)}{(1-\exp(2kl))(k_0^2-k^2)+4k_0^2k^2(1+\exp(2kl))^2} \tag{26}$$

$$R = \frac{(k_0^2+k^2)^2(1-\exp(-2kl))^2}{(1-\exp(2kl))(k_0^2-k^2)+4k_0^2k^2(1+\exp(2kl))^2} \tag{27}$$

$$R + T = 1$$

This case is quite astonishing.Clasically the particle can never go to region 3 as region 2 is classically forbidden to validate the eneergy conservation.But quantum mechanically there is a finite probability for the particle to tunnel through region 2 ,to be found at region 3. We can not define observables like momentum in region 2 & quantum mechanics asserts we need not to.What we can predict is there is a probability to find the particle in region 3.This phenomenon is termed as 'Tunneling'.Now,let $V_0 \to \infty$ and/or $l \to \infty$,from (26) & (27),we get $R \to 1$ & $T \to 0$ i.e. we approach the classical case where the particle is always reflected back.It can not tunnel through.So,we can conclude that a particle according to quantum mechanics can tunnel through any finite region of finite potential to be specific tunneling happens for any finite value of $V_0 l$.

3 Quantum Harmonic Oscillator:

A harmonic oscillator is a particle of mass m,moving under the potential $V(x) = \frac{1}{2}m\omega^2x^2$ .Classically its motion is described by

$$m\frac{d^2x}{dt^2} = -m\omega^2 x \tag{28}$$

with general solution $x = a\cos(\omega t - \omega t_0)$ & with total energy $\frac{1}{2}m\omega^2a^2$.So all positive values of E is allowed classically.

The quantum problem is to solve the differential equation:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2 = E\psi \tag{29}$$

Solution:

Lets substitute,$y = \sqrt{\frac{m\omega}{\hbar}}x$, equation (29) has now become

$$\frac{d^2\psi}{dy^2} = (y^2 - k) \tag{30}$$

where $k = \frac{2E}{\hbar\omega}$

We guess,$\psi(y) = A\exp(\frac{-y^2}{2})h(y)$

In terms of $h(y)$,the equation (30) has become:

$$\frac{d^2h}{dy^2} - 2y\frac{dh}{dy} + (k-1)h = 0 \tag{31}$$

Expanding $h(y)$ in power series and comparing coefficients of y^i,we get:

$$a_{i+2} = \frac{2i+1-k}{(i+2)(i+1)}a_i \tag{32}$$

So,if we know a_0 & a_1,two arbitrary constants,we can find all the coefficients by reccurence relation (32)

For large values of i,

$$a_{i+2} = \frac{2}{i}a_i$$

$$\Rightarrow h(y) = \sum_{even\ i} \frac{C}{(\frac{i}{2})!}y^i = C\exp(y^2)$$

$$\Rightarrow \psi(y) = C\exp(\frac{y^2}{2})$$

Clearly,$\psi(y)$blows up at infinity.The only way out is that the power series must terminate after finite number of terms.

$$\Rightarrow k = 2i_{max} + 1$$

$$= 2n + 1$$

$$\Rightarrow E_n = (n + \frac{1}{2})\hbar\omega \tag{33}$$

The ground state energy $E_0 = \frac{1}{2}\hbar\omega$.Its physical implication is that the particle has to oscillate in its lowest energy state too.And this happens according to heisenberg uncertainty principle.The energy is termed as 'Zero Point Energy'.

Equation (32) can be rewritten as

$$a_{i+2} = \frac{-2(n-i)}{(i+2)(i+1)}a_i$$

if n is even we choose $a_1 = 0$ to rule out the odd terms while in case of odd n,$a_0$is chosen to be 0 to rule out the even terms.The corresponding polynomial is called Hermite polynomial of degree n.(its highest power's coefficient is taken to be 2^n.So the quantum harmonic oscillator is described by the following apart from normalisation constant:

$$\psi_n(x) = AH_n(\sqrt{\frac{m\omega}{\hbar}}x)\exp(\frac{-m\omega}{2\hbar}x^2) \tag{34}$$

Equation (34) tells $\psi_{2n+1}(0) = 0$ i.e the particle can never be found at origin if it has $(2n + \frac{3}{2})\hbar\omega$ energy for $n \epsilon \mathbb{N}$.This result is diffrent from classical prediction too.

Let us get a deeper insight into the odd states.Suppose,we have a spring that can be streched but can never be compressed.the potential is described by the function $V(x) = \frac{1}{2}m\omega^2x^2 \ for \ x \geq 0$ & $V(x) = \infty \ otherwise$.It leads to the conclusion $\psi_n(0) = 0$ to make the function continuous at $x = 0$.All it implies that the particle has to be in an odd state with $(2m + \frac{3}{2})\hbar\omega$ energy.Here,

$$E_{n+1} - E_n = 2\hbar\omega \tag{35}$$

We can interpret this result physically.As the spring can not be compressed,the effective frequency of the spring get doubled which is manifested in (35).

4 Three Dimensional Quantum Harmonic Oscillator...A generalisation:

In case of 3 dimensional harmonic oscillator the particle moves under potential $V(r) = \frac{1}{2}m\omega^2r^2 = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$.

Now we have to solve the schr$ddoto$dinger equation:

$$\frac{-\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{36}$$

Seperation of variable leads to the solution

$$\psi(x,y,z) = A\exp(-\frac{m\omega}{2\hbar}r^2)H_n(\sqrt{\frac{m\omega}{\hbar}}x)H_k(\sqrt{\frac{m\omega}{\hbar}}y)H_l(\sqrt{\frac{m\omega}{\hbar}}z) \tag{37}$$

with energy

$$E_n = (n + k + l + \frac{3}{2})\hbar\omega$$

$$= (N + \frac{3}{2})\hbar\omega \tag{38}$$

The state is specified by three quantum numbers n,k,l.Degeneracy of the energy state

$$E_n = \begin{pmatrix} N+2 \\ N \end{pmatrix} \tag{39}$$

The generalisation in n dimension leads to the expression

$$E_N = (\sum n_i + \frac{n}{2}) \tag{40}$$

where $N = \sum n_i$.

Here the degeneracy is as follows:

$$d(N) = \begin{pmatrix} N+n-1 \\ N \end{pmatrix} \tag{41}$$

We conclude as the dimension goes up,the degeneracy of a particular energy state goes up.The system can attain a particular energy in various ways.

5 An electron constrained to move along an axis in field of a charge at origin:

The corresponding potetial for the problem is $V(x) = -\frac{e^2}{|x|}$.

Classically the charge would accelerate & it can acquire any energy.But quantum mechanics imposes quantisation condition on it.Here we look for only bound states i.e. $E < 0$.The equation governing its motion according to qm is:

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

$$= \left(\frac{-2mE}{\hbar^2} + \frac{2me^2}{\hbar^2|x|}\right)\psi$$

$$= \left(k^2 + \frac{P_0}{|x|}\right)\psi$$

where $k = \frac{\sqrt{-2mE}}{\hbar}$ & $P_0 = \frac{2me^2}{\hbar^2}$

For large values of x, $\frac{d^2\psi}{dx^2} \simeq k^2\psi$ with $\psi \simeq A\exp(-k|x|)$.On the other hand,potential is infinity at origin,it means that the particle cant cross the origin,hence the probability and therefore the wavefunction should go down to 0 at the origin.So we guess:

$$\psi(x) = Ax\exp(-k|x|)h(x) \tag{42}$$

Plugging the value of $\psi(x)$ in main equation we get a differential of $h(x)$:

$$2\frac{dh}{dx} - 2kh - 2kx\frac{dh}{dx} + x\frac{d^2h}{dx^2} = P_0 h(x) \tag{43}$$

Expanding $h(x)$ in power series and comparing the coefficients of x^i we get

$$a_{i+1} = \frac{P_0 + 2k(i-1)}{(i+2)(i+1)}a_i \tag{44}$$

where $h(x) = \sum_0^\infty a_i x^i$

For large i, $a_i \simeq \frac{2^i}{i!}a_0$ which in turn implies $h(x) = \exp(2x)$

$$\Rightarrow \psi(x) = Ax\exp(x)$$

This blows up at $x = \pm\infty$.So the power series must terminate after finite number of terms.

$$P_0 + 2k(i_{max} - 1) = 0$$

$$P_0^2 = 4k^2n^2$$

where $n = i_{max} - 1$

$$\Rightarrow E_n = \frac{-me^2}{2n^2\hbar^2} \tag{45}$$

This is the all wanted quantisation condition in accordance with qm.Later we will see equation (45) resembles the energy of an electron of hydrogen atom in its nth energy state.The only difference is degeneracy.In this case the particle can have this energy in one way,but in case of hydrogen atom this can be achieved many ways.

6 Angular Momenta :

It follows from the fact :$[L_i, L_j] = \imath\hbar\epsilon_{ijk}L_k$ & $[L^2, L_i] = 0$ that we can find simultaneous eigenfunction of L^2, L_z.Once the eigenfunction is chosen it wont be eigenfunction of L_x, L_y.Let that eigenfunction be $f(\theta, \phi) = g(\theta)h(\phi)$.

$$L_z f = kf$$

$$\Rightarrow -\imath\hbar\frac{\partial f}{\partial\phi} = kf$$

$$\Rightarrow -\imath\hbar\frac{dh}{d\phi} = kg$$

$$h(\phi) = A\exp(\imath\frac{k\phi}{\hbar}) \tag{46}$$

Now if we employ a rotation of 2π in space we come to same point.So,$h(\phi + 2\pi) = h(\phi)$.

$$\Rightarrow \frac{2\pi\imath k}{\hbar} = 2\pi\imath m$$

$$k = m\hbar \tag{47}$$

Equation (47) tells us z component of angular momenta can take only discrete values given by quantisation condition.Classically,L_z can take any value but quantum mechanics does not permit that.

Now we will look for eigenfunction of L^2.

$$L^2 f = af$$

$$\sin(\theta)\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial g}{\partial\theta}\right) - (m^2 - b\sin^2\theta)g(\theta) = 0$$

where $b = \frac{a}{\hbar^2}$

Let substitute $x = \cos\theta$;we will get:

$$(1-x^2)\frac{d^2g}{dx^2} - 2x\frac{dg}{dx} - \left(\frac{m^2}{1-x^2} - b\right) = 0 \tag{48}$$

Let us look for the solution when x is so large that we can rewrite (48) as:

$$(1-x^2)\frac{d^2g}{dx^2} - 2x\frac{dg}{dx} + b = 0 \tag{49}$$

Expanding $g(x)$ in power series & comparing coefficients of x^i,we get

$$a_{i+2} = \frac{i^2 + i - b}{(i+2)(i+1)}a_i$$

where $g(x) = \sum_0^\infty a_i x^i$

For large i,$a_i \simeq a_{i-2}$

$$\Rightarrow g(x) \simeq a_0(1 + x + x^2 + \ldots\ldots)$$

which clearly diverges.So the power series must terminate after finite number of terms.

$$b = i_{max}^2 + i_{max} = l(l+1)$$

$$\Rightarrow L^2 f = l(l+1)\hbar^2 f$$

$$\Rightarrow |\overrightarrow{L}| = \sqrt{l(l+1)}\hbar \tag{50}$$

Classically,modulus of angular momenta can take any value but qm imposes quantisation condition on it given by (50).

Equation (48) can now be written as :

$$(1-x^2)\frac{d^2g}{dx^2} - 2x\frac{dg}{dx} - \left(\frac{m^2}{1-x^2} - l(l+1)\right) = 0 \tag{51}$$

The solution to the equation is:

$$g(x) = (1-x^2)^{\frac{|m|}{2}} \left(\frac{d}{dx}\right)^{|m|} P_l(x) \tag{52}$$

where $P_l(x) = \left(\frac{d}{dx}\right)^l (1-x^2)^l$

$$g(\theta) = P_l^m(\cos\theta) \tag{53}$$

Now $P_l(\cos\theta)$ is a polynomial of degree l in $\cos\theta$.So $P_l^m(\cos\theta) = 0 \; if \; m > l$

So,for agiven value of l,m can take values between -l to +l including both of them i.e $(2l+1)$ values in all.

7 Hydrogen atom:

For any spherically symmetric potential,we look for seperable solution $\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$ with seperation constant $l(l+1)$.By previous analysis $Y(\theta,\phi) = A\exp(\imath m\phi)P_l^m(\cos\theta)$ where $m = 0, \pm1, \pm2, ... \pm l$.The radial part reduces to

$$\frac{-\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right)u = Eu \tag{54}$$

if we substitute $u(r) = rR(r)$

We look for bound state i.e $E < 0$.Let $k^2 = \frac{-2mE}{\hbar^2}$ & $p = kr$ & $P_0 = \frac{2me}{k\hbar^2}$.The equation (54) reduces to:

$$\frac{d^2u}{dp^2} = \left(1 - \frac{P_0}{p} + \frac{l(l+1)}{p^2}\right)u \tag{55}$$

Checking the assymptotic behaviour by letting $p \to \infty$ & $p \to 0$,we guess

$$u(p) = Dp^{l+1}\exp(-p)v(p)$$

With this substitution equation(55) has now become

$$p\frac{d^2v}{dp^2} + 2(l+1-p)\frac{dv}{dp} + (P_0 - 2(l+1))\,v = 0$$

Expanding $v(p)$ in power series & comparing coefficients of x^i,we get

$$a_{i+1} = \frac{-P_0 + 2(i+l+1)}{(i+1)(2l+2+i)}a_i \tag{56}$$

For large value of i,$a_i \simeq \frac{2^i}{i!}a_0$ which implies $u(p) = \exp(p)p^{l+1}$.If the series is infinite u(p) blows up.So,the power series must terminate after finite number of terms.

$$\Rightarrow 2(i_{max} + l + 1) = P_0$$

Define principle quantum number $n = (i_{max} + l + 1)$.

$$P_0 = 2n$$

$$\Rightarrow E_n = \frac{-me^4}{2\hbar^2 n^2} \tag{57}$$

This is the allowed energy level for hydrogen atom this owes to the fact that hydrogen spectrum is discrete rather than being continuous.(The fine structure is due to relavistic correction).

From definition we can say,for a given value of n, l can take values from 0 to n-1.On the other hand,m can take value from -l to l.So the degeneracy of nth state is

$$d(n) = \sum_{l=0}^{n-1}(2l+1) = n^2$$

Here l is called Azimuthal quantum number & m is called magnetic quantum number.

8 Relativistic Schr$\ddot{o}$dinger Equation:

8.1 Klein Gordon Model:

We recall we got the schr$\ddot{o}$dinger equation by writing $E = \frac{p^2}{2m}$ as an operator equation.But it is correct only in non-relativistic realm.According to relativity,

$$E^2 = m_0^2 c^4 + p^2 c^2$$

We can write off the schr$\ddot{o}$dinger equation in following manner

$$\sqrt{m_0^2 c^4 + \hbar^2 c^2 \nabla^2}\psi = \imath\hbar\frac{\partial\psi}{\partial t} \tag{58}$$

But the problem with (58) is that it is asymmetric in terms of derivatives with respect to space and time i.e (58) is not a covariant equation,hence it is rejected.

The next proposal came from Klein Gordon

$$\hat{H}^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial t^2}$$

Taking the complex conjugate of the equation substracting one from other we get

$$\frac{\imath\hbar}{2m}\nabla(\psi\nabla\psi^* - \psi^*\nabla\psi) = \frac{\imath\hbar}{2mc^2}\frac{\partial}{\partial t}(\psi\partial_t\psi^* - \psi^*\partial_t\psi)$$

So,Klein Gordon admits a probability function

$$p = \frac{\imath\hbar}{2mc^2}(\psi\partial_t\psi^* - \psi^*\partial_t\psi) \tag{59}$$

which can be negative too.Since probability cant be negative,the Klein Gordon model is ruled out.

8.2 The Dirac Equation:

Dirac began to find an equation which is covariant as well as admits positive definite probability.So he proposed:

$$H_{Dirac} = c\overrightarrow{\alpha}.\overrightarrow{p} + \beta m_0 c^2 \tag{60}$$

Now we will find the condition for which

$$H_{Dirac}^2 = H^2$$

This translates into:

$$\alpha_i\alpha_k + \alpha_k\alpha_i = 2\delta_{ik}1 \tag{61}$$

$$\alpha_i\beta + \beta\alpha_i = 0 \tag{62}$$

$$\beta^2 = 1 \tag{63}$$

These induce us to think α_i, β are matrices.Now,

$$\det(\alpha_i\beta) = (-1)^n \det(\beta\alpha_i)$$

$$\Rightarrow n\ is\ even$$

Simple manipulation reveals $tr(\alpha_i) = 0$.
For n=2 we can have at most 3 linearly independent traceless matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

So we try n=4.

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}$$

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

α_i, β indeed satisfies (61),(62),(63).So the Dirac equation looks like this:

$$\begin{pmatrix} m_0c^2 & -\imath\hbar\overrightarrow{\sigma}.\overrightarrow{\nabla} \\ -\imath\hbar\overrightarrow{\sigma}.\overrightarrow{\nabla} & -m_0c^2 \end{pmatrix}\psi = \imath\hbar\frac{\partial\psi}{\partial t} \tag{64}$$

Here we see $\psi(x)$ is not a scalar now,rather it has now become a spinor of four componect whose physical signicance will be revealed soon.Taking complex conjugate $\psi^\dagger$,and a bit of matrix algebra reveals that Dirac model admits a probability $\psi^\dagger\psi = \sum\psi_i^*\psi$ with conserved probability density $c\psi^\dagger\psi$.

Now we will show spin is automatically manifested in Dirac model.It represents particle with spin $\frac{1}{2}$.

$$[L_i, H] = \begin{pmatrix} 0 & \hbar^2c(\overrightarrow{\sigma}\times\overrightarrow{\nabla})_i \\ \hbar^2c(\overrightarrow{\sigma}\times\overrightarrow{\nabla})_i & 0 \end{pmatrix}$$

We see,$[L_z, H] \neq 0$.We know $\frac{d}{dt}\overline{L_z} \propto \overline{[L_z, H]}$ i.e L_z is not conserved quantity.But for a free particle angular momentum should be conserved.All it implies that there is some other form of angular momentum intrinsic to particle.This is what we know as 'Spin'.We take

$$S_i = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}\frac{\hbar}{2}$$

and use the fact $\overrightarrow{\sigma}\times\overrightarrow{\sigma} = 2\imath\overrightarrow{\sigma}$,we get $[L_i + S_i, H] = 0$

$$\Rightarrow \frac{d}{dt}\overline{L_i + S_i} = 0$$

So the angular momentum is conserved.Now the eigenvalues of S_z in units of $\hbar$ is $\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}$.We interpret the result in following manner:ψ_i represents particle and antiparticle with spin $\frac{1}{2}$ & $-\frac{1}{2}$ with energy eigenvalue $E = \pm\sqrt{m_0^2c^4 + p^2c^2}$.From here we can see $E \geq m_0c^2$ *or* $E \leq -m_0c^2$.The $m_0c^2 > E > -m_0c^2$is termed as forbidden energy.The particle cant have any energy between those two values.But still particle can tunnel through this region to reach a place where it has no finite minimum energy,a physically unacceptable situation.So Dirac proposed that all the energy levels below $-m_0c^2$ are occupied by particles and thereby ruled out the possibility of tunneling, exploiting Pauli's Exclusion Principle.

9 Search for Extra Dimension:

In the beginning of 20th century Gunnar Nordstrom,Theodor Kaluza and Oscar Klein extended general relativity to include an extra dimension.To make sense of this radical proposal Klein proposed to curl up extra spatial dimension.Mathematically speaking,the extra dimension is suggested to be compactified within such a small radius that we can not feel or measure it.The end result is that we get back our familiar $3+1$ dimensional world with a tiny 'ball' of extra dimension associated with each point of our space.What does quantum mechanics predict about a free in such a space with curled up dimension?Let us take a two dimensional plane with normal X axis and Y direction compactified with radius r.

[We will do following calculation in units such that $\hbar = 1$ & $c = 1$]

We know spatial part of ψ representing a free particle is

$$f(x, y) = \exp(\imath p_x x) \exp(\imath p_y y)$$

Now curled up Y impose the following condition on $f(x, y)$

$$f(x, y + 2\pi r) = f(x, y) \tag{65}$$

Equation(65) implies $p_y r = n$;which in turn implies

$$p_y = \frac{n}{r} \tag{66}$$

So one of the physical implication of curling up is momentum along this dimension being quantised and so the energy.From Einstein's relation we get,

$$m^2 = m_0^2 + \frac{n^2}{r^2} + p_x^2 \tag{67}$$

where $m_0$is rest mass of the particle.If we let $r \to 0$,the energy blows up.It implies that infinite amount of energy is required to squeeze any dimension.

Now consider a situation from one dimensional world.What would be the energy of the particle if we can not detect i.e enter into the extra dimension?The energy $\frac{n^2}{r^2}$ can not be manifested directly.Rather it will show up as states of massive particle.In particular, a massless state in the higher dimensional theory will show up in lower dimensional theory as a tower of massive states.This is known as Kaluza-Klein Tower.If we see the (67) carefully,we can only detect p_x^2.So from lower dimensional point of view

$$m_0'^2 = m_0^2 + \frac{n^2}{r^2} \tag{68}$$

where m_0 is 0th massless state and m_0' is new rest mass.According to this theory the number of particles is infinite.String theory does indeed admit that.This tower of particles induces us to explore extra curled up dimension as well as to search for new particles.An observer in the lower dimensional word witnessing the outcome of the collision would see imbalance of energy and momentum.The missing energy is a signature of Kaluza Klein particle.Not to say,this is the way the existense of Neutrino and Graviton is inferred in collider experiments.Had it been like that the dimensionsion are not curled up the unification happens.Because the dimension is curled up,a particle shows up different massive mass state.

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References

[1] David J.Griffith,Introduction to Quantum Mechanics(2008)

[2] B.Thaller,The Dirac Equation(1992)

[3] R.Shankar,Principles of Quantum Mecanics(1994)