MODULE 12

Quantum Mechanics – free particle, Dirac Delta Function, 1D Potential

The free particle

For a free particle, the potential V(x) = 0 every where

substituting this value inthe Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V\psi=E\psi \qquad [1]$$

where m is the mass of the free particle, ψ, the wavefunction representing the state of the particle, V the potential experienced by the particle and E its total energy.

Putting V = 0 *(as free particle is one not affected by a repulsive or attractive potential)*we get

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi \qquad [2]$$

Xing [2] by $-\frac{2m}{\hbar^2}$ $$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \qquad [3]$$

If we substitute $$k = \frac{\sqrt{2mE}}{\hbar} \qquad [4]$$

we get

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad [5]$$

This is the form of Schrodinger equation for a free particle. The solution for the above equation can be

$$\psi(x) = A\,e^{ikx} + Be^{-ikx} \qquad [6]$$

The first term in equation [6] represents a wave travelling to right and second term represent a wave travelling to left.

But

$$k = \frac{\sqrt{2mE}}{\hbar} \qquad \therefore k^2 = \frac{2mE}{\hbar^2}$$

$$\therefore E = \frac{\hbar^2 k^2}{2m} \qquad [7]$$

The states of a free particle are propagating waves with wavelength

$$\lambda = \frac{2\pi}{k} \qquad [8]$$

But the de Broglie relation $p = \frac{h}{\lambda}$

where p is the momentum of the free particle

But $$p = \frac{h/2\pi}{\lambda/2\pi} = \frac{\hbar}{\left(1/k\right)}$$ $$k = \frac{2\pi}{\lambda}$$

$$\therefore p = \hbar k \qquad [9]$$

The speed of such a particle in given by

$$v = \frac{\omega}{k}$$

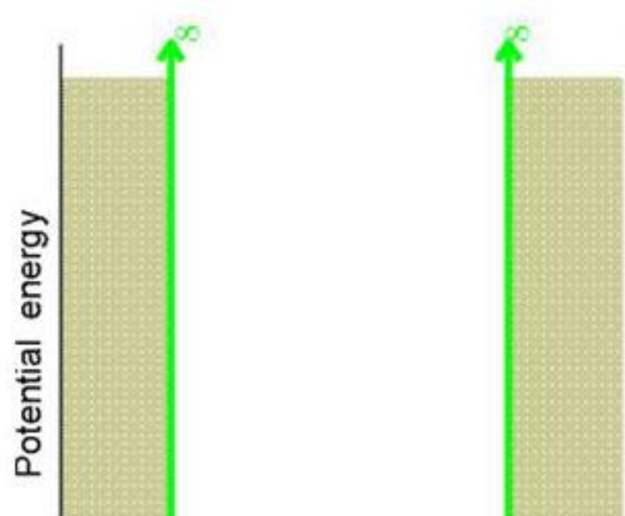
But $\hbar\omega = \dfrac{\hbar^2 k^2}{2m}$ $\qquad \therefore \omega = \dfrac{\hbar k^2}{2m}$

$$v = \frac{\hbar k^2/2m}{k} = \frac{\hbar k}{2m}$$

According to quantum theory the speed of a free particle

$$v_{quantam} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}} \qquad [10]$$

A wave packet is a superposition of sinusoidal waves whose amplitude is modulated by phase ϕ.



A free particle is represented by a wave packet which is formed by addition of sinusoidal waves. Sinusoidal wave is formed by addition of sinusoidal waves. Sinusoidal waves add to form a wave packet. Individual waves forming the packet travels but the packet travels with a group velocity. The velocity of the envelope is called group velocity while individual velocity of the waves are called phase velocity or wave velocity which do not make any physically observable effects.

The wave function representing a free particle is given by

$$\psi(x,t) = A\, e^{ikx} \qquad [11]$$

For normalization, the condition is

$$\int_{-\infty}^{+\alpha} \psi^* \psi \, dx = \perp$$

$$\int_{-\infty}^{+\alpha} Ae^{-ikx}.Ae^{+ikx} dx = |A|^2 \int_{-\infty}^{+\infty} dx = \infty$$

The wave function f a free particle are not normalizable. Ie the free particle cannot exist in a stationary state.

The Delta Function Potential

Bound states and scattered state

The one dimensional schrodinger equation is given by

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+V\right]\psi = E\psi \qquad [12]$$

Two kinds of solution are possible for this equation if E<V where E is the total energy of the particle and V is the prevailing potential in the region through which the particle is travelling in this case the particle gets trapped in the potential and this state is called bound state. For example in the case of electron inside a hydrogen atom, its kinetic energy is less than that of the attraction by the nucleus. Hence it can only admit bound state solution. But if E>V, In such a case a particle coming from infinity slows down or accelerates near d potential depending an its type and returns to infinity. This state is called scattered state. Some potentials admit only bound states, some allow only scattered states and same permit both kinds of solutions.

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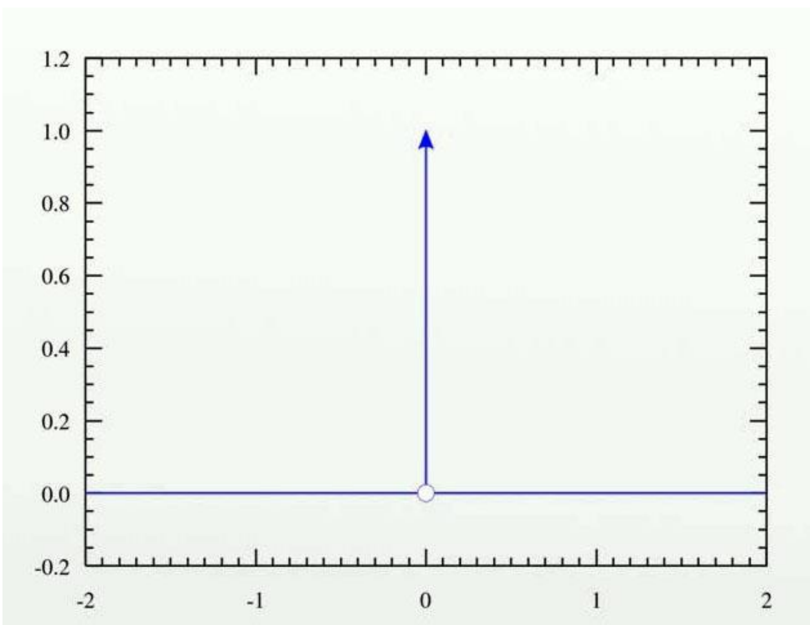
Dirac Delta Function (DDF)

DDF is an infinitely high and infinitesimally narrow spike at the origin and is represented mathematically as



$$\left.\begin{array}{l}\delta(x) = 0 \ \text{ if } \ x \neq 0 \\ \delta(x) = \infty \ \text{ if } \ x = 0\end{array}\right\} \qquad [13]$$

Also $\int_{-\infty}^{+\infty} \delta(x)dx = 1$ [14]

$$f(x)\delta(x-a) = f(a)\,\delta(x-a) \qquad [15]$$

and

$$\int_{-\infty}^{+\infty} f(x)\,\delta(x-a)dx = f(a) \qquad [16]$$

Consider a potential form

$$V(x) = -\alpha\,\delta(x) \qquad [17]$$

The Schrodinger equation is given by

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V\right]\psi = E\psi \qquad [18]$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi \qquad [19]$$

For bound states $E < 0$ and for scattered States $E > 0$

For region $x < 0$ $\quad V(x) = 0$ [20]

$\therefore$ Schrodinger equation becomes

$$\frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi = k^2\psi \qquad [21]$$

Where $k^2 = \frac{-2mE}{\hbar^2}$ $\qquad k = \frac{\sqrt{-2mE}}{\hbar}$ [22]

As E < 0 ie E is negative, so k will be real and positive.

The general solution to equation 10 is

$$\psi(x) = Ae^{-kx} + Be^{kx} \qquad [23]$$

But x varies from O to $-\infty$

In this lint $e^{kx} \to \infty$ for $x = -\infty$ and there the probability $\psi^{*}\psi$ is not defined

This can be avoided by choosing A = 0

$$\therefore \psi(x) = Be^{kx} \qquad [24]$$

In the region x > 0 V(x) = 0 [25]

Hence solution will be

$$\psi(x) = Fe^{-kx} \quad \text{for } x > 0 \qquad [26]$$

e^{+kx} is avoided as $x \to \infty$ $e^{kx} \to \infty$

But in quantum mechanics ψ should be well behaved

1. ψ should be always continuous

2. $\frac{d\psi}{dx}$ is continuous except where $V(x) = \infty$ [27]

If we apply 1st boundary condition

$Be^{k.0} = Fe^{-k.0}$ At x = 0

ie B = F

$$\therefore \quad \begin{aligned} \psi(x) &= Be^{kx} \quad x \leq 0 \\ \psi(x) &= Be^{-kx} \quad x \geq 0 \end{aligned} \qquad [28]$$

By integrating the schrodinger equation from –E to +E and then taking limits $E \to 0$

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

$$= E\int_{-E}^{+E}\psi(x)dx \qquad [29]$$

The first integral evaluates to $\frac{d\psi}{dx}$ and should apply limits and find upper limit minus lower limit denoted by

$$\Delta\frac{d\psi}{dx} = \left.\frac{\partial\psi}{\partial x}\right|_{x=+E} - \left.\frac{\partial\psi}{\partial x}\right|_{x=-E} \qquad [30]$$

The last integral

$$\int_{-E}^{+E}\psi(x)dx = 0 \qquad [31]$$

With in the limit $\in \to 0$

$$\therefore \Delta\frac{d\psi}{dx} = \frac{2m}{\hbar^2}\underset{\in\to 0}{\mathrm{Lin}}\int_{-E}^{+E}V(x)\psi(x)dx \qquad [32]$$

Substituting for $V(x) = -\alpha\, d(x)$ [33]

$$\operatorname{Lin}_{E\to 0} \int_{-E}^{+E} -\alpha\,\delta(x)\,\psi(x)\,dx = -\alpha\,\psi(0)$$

$$\therefore \Delta\frac{d\psi}{dx} = \frac{-2m\alpha}{\hbar^2}\psi(0) \qquad [34]$$

Recalling equation (17)

$$\frac{d\psi}{dx} = -Bke^{-kx} \qquad x > 0 \qquad [35]$$

$$\frac{d\psi}{dx} = -+Bk.e^{kx} \qquad x < 0 \qquad [36]$$

$$\left.\frac{d\psi}{dx}\right|_{+0} = -Bk \qquad \left.\frac{d\psi}{dx}\right|_{0-} = +Bk\} \qquad [37]$$

$$\therefore \Delta\frac{d\psi}{dx} = -Bk - Bk \qquad = -2Bk \qquad [38]$$

Substituting is eqn. (23)

$$-2Bk = \frac{-2md}{\hbar^2}\psi(0) \qquad [39]$$

Substituting for x = 0 $\qquad \psi(0) = B$ [40]

$$k = \frac{m\alpha}{\hbar^2} \qquad [41]$$

But $k = \frac{\sqrt{-2mE}}{\hbar}$ from eqn. (11)

$$\therefore E = \frac{-\hbar^2k^2}{2m} = \frac{-\hbar^2m^2\alpha^2}{2m\,\hbar^2}$$

$E = \frac{-m\alpha^2}{2\hbar^2}$ eqn for Energy

Normalizing ψ

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = \int_{-\infty}^{0} B^2 e^{2kx} dx + \int_{0}^{\infty} B^2 e^{-2kx} dx$$

This can be written as

$$\int_{-\infty}^{+\alpha} |\psi(x)|^2 \, dx = 2|B|^2 \int_{0}^{\infty} e^{-2kx} dx$$

$$= 2|B|^2 \left[\frac{e^{-2kx}}{-2k}\right]_0^\infty$$

Applying limits we get

$$\int_{-\alpha}^{+\alpha} |\psi(x)|^2 \, dx = \frac{|B|^2}{k} = 1$$

$|B|^2 = k$ or $|B| = \sqrt{k}$

$\text{ie} |B| = \frac{\sqrt{mx}}{\hbar}$ $\because k = \frac{mx}{\hbar^2}$

$\therefore \psi(x) = \frac{\sqrt{mx}}{\hbar} e^{\frac{-mx}{\hbar^2}x}$ Wave function [42]

Energy $E = \frac{-m\alpha^2}{2\hbar^2}$ [43]

ie Regard less of its strength a delta function potential has one bound state.

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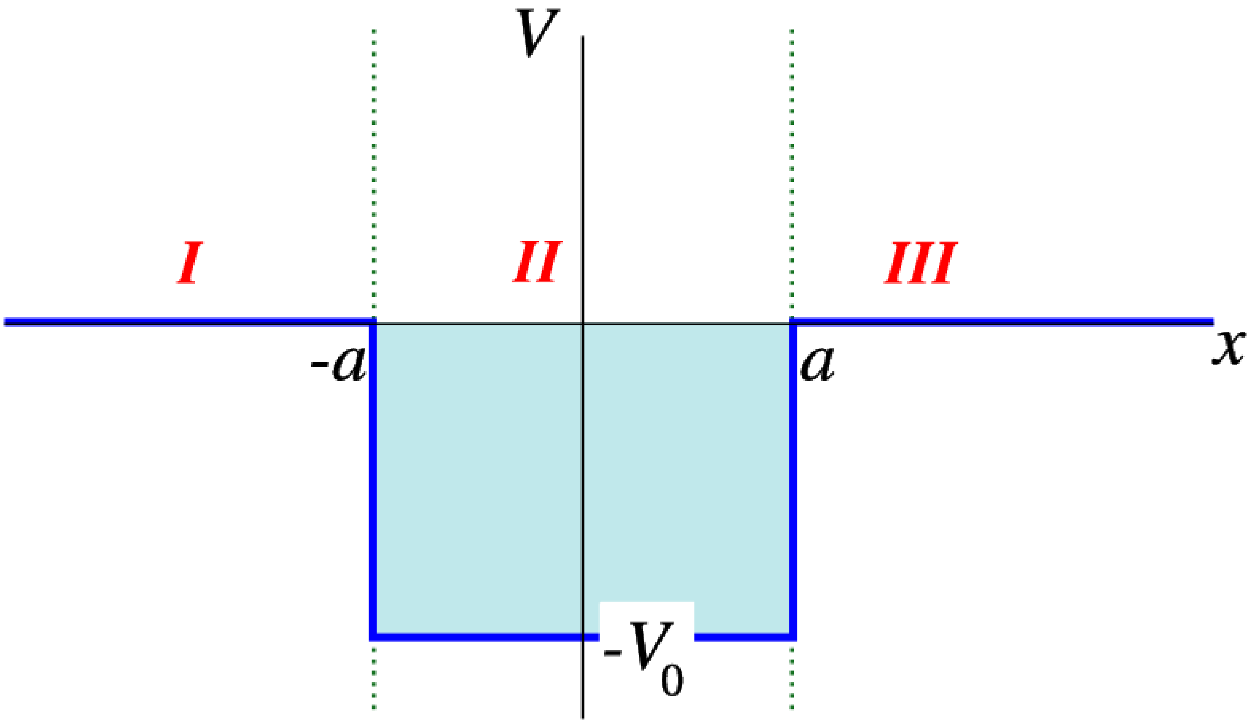
Finite square well potential



One dimensional square well potential is defined as

$$\left.\begin{array}{lll} V(x)=0 & x<-a & \text{I region} \\ V(x)=-V_0 & -a<x<a & \text{II region} \\ V(x)=0 & x>a & \text{III region} \end{array}\right\} \qquad [44]$$

Consider the case E < 0 (bound states) A particle trapped in a well cannot enter region I and region III classically.

The Schrodinger equation for the region are

$$\frac{-\hbar^2}{2m}\frac{d^2U}{dx^2} = Eu \qquad \text{I and III regions} \qquad [45]$$

$$\frac{-\hbar^2}{2m}\frac{d^2U}{dx^2} - V_0U = EU \qquad \text{II region} \qquad [46]$$

$$\text{Let } \alpha^2 = \frac{2mE}{\hbar^2} \qquad [47]$$

$$\beta^2 = \frac{2m}{\hbar^2}(E + V_0) \qquad [48]$$

If E > 0 *ie.* for scattered states

$$\frac{d^2\psi}{dx^2} = \frac{2mE}{\hbar^2}\psi \qquad [49]$$

$$\text{E is +ve} \quad k = \frac{\sqrt{2mE}}{\hbar} \qquad [50]$$

$$\text{So that } d\frac{d^2\psi}{dx^2} = -k^2\psi$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad [51]$$

General solution is

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad \text{for } x < 0 \qquad [52]$$

$$\psi(x) = Fe^{ikx} + Ge^{-ikx} \qquad \text{for } x > 0 \qquad [53]$$

Also $B = \frac{i\beta}{1-i\beta}A$ and $F = \frac{1}{1-i\beta}A$ [54]

Where $\beta = \frac{mx}{\hbar^2 k}$

Reflection coefficient and Transmission Coefficient are

$|R| = \frac{\beta^2}{1+\beta^2}$ [55] $T = \frac{1}{1+\beta^2}$ [56]

and $R + T = 1$ [58]

$$\frac{d^2U}{dx^2} - \alpha^2 U = 0 \quad [59]$$

$$\frac{d^2U}{dx^2} + \beta^2 U = 0 \quad [60]$$

The solution for the above equation are

$$[61] \leftarrow U_I(x) = C e^{\alpha x} \qquad -\infty < x < -a$$

$$[62] \leftarrow U_{III}(x) = D\, e^{-\alpha x} \qquad [63] \leftarrow U_{III}(x) = D\, e^{-\alpha x}$$

$$[64] \leftarrow U_{II}(x) = A\cos\beta x + B\sin\beta x \qquad -a < x < a$$

For the well behaviour of the wave function

$$[65] \leftarrow U_I = U_{II}\,|_{x=-a} \qquad [66] \leftarrow U_{II} = U_{III}\,|_{x=a}$$

$$[67] \leftarrow \frac{dU_I}{dx} = \frac{dU_{II}}{dx}\,\Big|_{x=-a} \qquad [68] \leftarrow \frac{dU_{II}}{dx} = \frac{dU_{III}}{dx}\,\Big|_{x=a}$$

Applying in eqn. (59)

$$C\,e^{-\alpha a} = A\cos(-\beta a) + B\sin(-\beta a)$$

$$Ce^{-\alpha a} = A\cos\beta a - B\sin\beta a \qquad [69]$$

$$\text{as}\sin(-\theta) = -\sin\theta \qquad \cos(-\theta) = \cos\theta$$

Applying in equations

$$C\alpha e^{\alpha x}\,\big|_{\text{at } x=-a} = \left[(A\beta(-)\sin\beta x) + B\beta\cos\beta x\right]_{x=-a}$$

$$\text{ie}\; C\alpha e^{-\alpha a} = A\beta\sin\beta a + B\beta\cos\beta a \qquad [70]$$

Applying in eqn. (12)

$$De^{-\alpha a} = A\cos\beta a + B\sin\beta a \qquad [72]$$

$$-D\alpha e^{-\alpha a} = -A\beta \text{Sin}\beta a + B\beta\cos\beta a \qquad [73]$$

Adding and subtracting the above equations

$$\left.\begin{aligned}(C+D)e^{-\alpha a} &= 2A\cos\beta a \quad 18(a)\\ (C-D)\alpha e^{-\alpha a} &= 2B\beta\cos\beta a \quad 18(b)\\ (C-D)e^{-\alpha a} &= -2B\sin\beta a \quad 18(c)\\ (C+D)\alpha e^{-\alpha a} &= 2A\beta\sin\beta a \quad 18(d)\end{aligned}\right\} \qquad [74]$$

Case 1 if $C + D \neq 0 \quad A \neq 0$

$$\left.\begin{aligned}\alpha &= \beta\tan\beta a \quad 18(d)/18(a)\\ -\alpha &= \beta\cot\beta a \quad 18(b)/18(c)\end{aligned}\right\} \qquad [75]$$

$$\beta\tan\beta a = -\beta\cot\beta a$$

$$\text{ie}\,\frac{\sin\beta a}{\cos\beta a} = \frac{-\cos\beta a}{\sin\beta a} \qquad [76]$$

$$ie \sin^2 \beta a + \cos^2 \beta a = 0 \qquad [77]$$

This result is absurd. This can be avoided if we take B = 0 *ie.* C – D = 0

$\therefore C = D$ and $B = 0$ **One set of solution**

Case 2

$$C - D \neq 0 \quad B \neq 0 \qquad [78]$$

Here also $\cos^2 \beta a + \sin^2 \beta a = 0$

This situation can be avoided by taken

A = 0 C = -D

Eigen Function

Two sets of solution are

$$C = D \frac{\alpha = \beta \tan \beta a}{\text{and } B = 0} \qquad D = Ae^{\alpha a} \cos\beta a \qquad [79]$$

I set of wave function are

$$U_n^I(x) = \left[Ae^{\alpha_n a} \cos\beta_n a\right] e^{\alpha_n x}$$

$$U_n^{II}(x) = A \cos\beta_n x$$

$$U_n^{III}(x) = \left[Ae^{\alpha_n a} \cos\beta_n a\right] e^{-\alpha_n x}$$

For second set

$$C = -D \qquad A = 0 \qquad D = Be^{\alpha a} \sin \beta a \qquad [80]$$

$$\left.\begin{array}{l} U_n^{I}(x) = \left[-Be^{\alpha na}\sin\beta_n a\right]e^{\alpha_n x} \\ U_n^{II}(x) = B\sin\beta_n x \\ U_n^{III}(x) = \left[Be^{\alpha_n a}\sin\beta_n a\right]e^{-\alpha_e x} \end{array}\right\} \quad [90]$$

First set of solutions satisfy

$$U_n(x) = U_n(-x) \quad [91]$$

There function here even parity and for the second set

$$U_n(x) = -U_n(-x) \quad [92]$$

There functions here odd parity.

Eigen values of energy

$$\beta^2 = \frac{2m}{\hbar^2}(E + V_0) \quad [93]$$

$$\alpha^2 = \frac{2mE}{\hbar^2} \quad [94]$$

$$\therefore \frac{2mV_0}{\hbar^2} = \alpha^2 + \beta^2 \quad [95]$$

Xing by a^2

$$\frac{2mV_0 a^2}{\hbar^2} = \left(\alpha^2 + \beta^2\right)a^2 \quad [96]$$

Putting $\Delta = \frac{\hbar^2}{2ma^2}$ [97]

$$\frac{V_0}{\Delta} = \left(\alpha^2 + \beta^2\right)a^2 \qquad [98]$$

But $\alpha = \beta \tan \beta a$ [99]

$$\therefore \frac{V_0}{\Delta} = \left(\beta^2 \tan^2 \beta a + \beta^2\right) \qquad [100]$$

$$= (\tan^2 \beta a + 1)\beta^2 a^2$$

$$= \sec^2 \beta a \beta^2 a^2$$

$$= \frac{\beta^2 a^2}{\cos^2 \beta a} \qquad [101]$$

$$\cos^2 \beta a = B^2 a^2 \left(\frac{\Delta}{V_0}\right) \qquad [102]$$

$$\text{Or } |\cos\beta a| = \beta a \left(\frac{\Delta}{V_0}\right)^{1/2} \qquad [103]$$

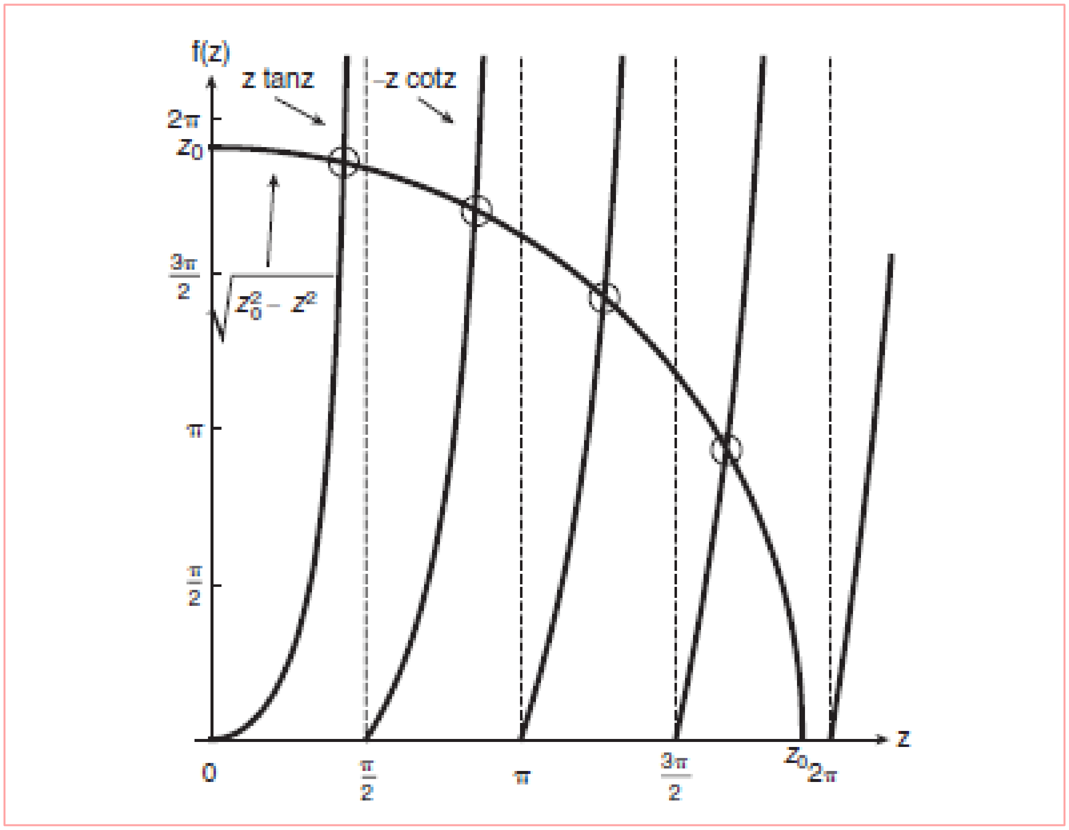
Case 2 $\alpha = -\beta \cot \beta a$ [104]

$$\frac{V_0}{\Delta} = \beta^2 (1 + \cot^2 \beta a) a^2 \qquad [105]$$

$$= B^2 a^2 \ \mathrm{cosec}^2 \beta a \qquad [106]$$

$$\frac{V_0}{\Delta} = \frac{\beta^2 a^2}{\sin^2 \beta a} \qquad [107]$$

$$\therefore |\sin \beta a| = \beta a \left(\frac{\Delta}{V_0}\right)^{1/2} \qquad [108]$$



Only at intersection points the equations (39) and (44) are valid. β can take only discrete values given by intersecting points. $\frac{V_0}{\Delta}$ is a measure of the strength of the potential. Thus the energies if the particle have to be quantized.

https://www.youtube.com/watch?v=E7RMF9cRxls

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