Solution for Gauss Circle problem for integer value of R and it's application in finding the number of quantum states available to a particle in 2-D box

Abstract: Determination of number of integer pairs of (x,y) coordinates in the region bounded by the circle of radius R is gauss circle problem. As we know the number of energy states available below an energy level is for a particle in the box problem is the number of non-zero integer values of n_x *and* n_y satisfying the equation $n_x^2 + n_y^2 \le N$, where $E_N = N \cdot E_1$. In this paper to evaluate the number of quantum states available by considering energy levels in 2-D as spatial coordinates and hence solving the gauss circle problem and calculating the integer pairs inside the circle in 1st quadrant a more precise answer is abstracted. In this paper program for solving the gauss circle problem for an integer value of radius and evaluation of quantum states available is presented. The data achieved by the program is further analysed graphically.

Introduction:

Gauss circle problem: Determination of number of integer pairs of (x,y) coordinates in the region bounded by the circle of radius R is gauss circle problem.[1]

Considering a circle with a radius R, furthermore considering the value of R to be an integer as N which is energy level is quantised and is an integer. Now, constructing lines parallel to the X-axis with a separation of unit distance with each other and repeating this procedure for Y-axis. The number or intersections of these lines on the plane are the integer pairs of x and y coordinates. In order to solve this problem we need to calculate the number of intersections inside the circle.

First we consider 1st quadrant and then, Now varying the x coordinate from R to 0 by the continuously decrementing it by 1 and calculating the y coordinate for the given x coordinate

$x^2 + y^2 = R^2$ by the equation of circle

We get, $y = \sqrt{(R^2 - x^2)}$

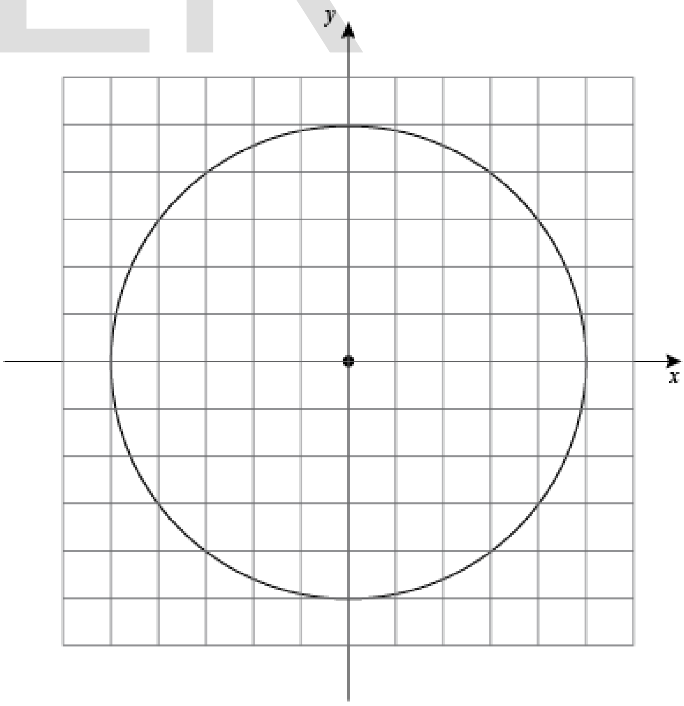
In this x which we are considering is an integer, y calculated from this may or may not be an integer. For clear understanding let us consider some arbitrary value of y, let y=2.45. in the x-y plane it means that when the circle's X coordinate reaches from R to (R-1) then there are 2 lines parallel to X axis and which are intersecting with (R-1) lines parallel to Y axis. Therefore, number of intersection which is equal to the number of integer pairs of x and y in the above case is

$n_i = (R - i) \cdot [y_i]$

Where [n] represents, integer part of n.

Now coming from (R-1) to (R-2) suppose we get the value of y to be 3.25, that is we have 3 lines parallel to X-axis, but we have considered the intersection with 2 lines before while we travelled from R to (R-1). In order to neglect the previously calculated intersections we subtract $[y_i] - [y_{i-1}]$, by doing this we consider only new line or lines parallel to X-axis introduced.

Therefore, $n_i = (R - i) \cdot \left(\left[\sqrt{(R^2 - (R-i)^2)}\right] - \left[\sqrt{(R)^2 - x^2)}\right] \right)$



Where n_i is the number of intersections in ith step

So for R steps we have.

$N = \sum_{i=1}^{R} (R - i) \cdot ([y_i] - [y_i - 1]),$

Where N is the number of intersections occurred in 1st quadrant

As the center of the circle is origin and by the property of symmetry of circle, it is fair to consider the number of intersections occurred in 2nd, 3rd. 4th and that of 1st are same.

Also there are intersections on the axis which are not considered in the above analysis. There are 2R lines intersecting each axis (R on each side) as the origin of the circle is considered to be at (0,0), also both axis intersect with each other at (0,0).

Therefore number of intersections on occurred on axis is given by

$S = 4R + 1;$

Now total number of intersections between lines parallel to X-axis and lines parallel to Y-axis which are spaced at unit distance (T) inside the circle of radius R is given by

T=S+4N

$$T= (4R+1) +4.\left(\sum_{i=1}^{R}(R-i)\cdot\left(\left[\sqrt{(R^2-(R-i)^2)}\right]-\left[\sqrt{(R^2-(R-i-1)^2)}\right]\right)\right)$$

Henceforth we have calculated the number of integer pairs of x and y coordinates inside the circle of radius R, R being an integer.

$$v(x,y) = 0$$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main.c
#include <stdio.h>
#include<conio.h>
#include<math.h>
void main()
{
    int y,y1=0,y2=0,i,R,s=0,T=0;
    for(R=1;R<=15;R++)
    {
        s=0;
        for(i=1;i<=R;i++)
       {
        int y1=sqrt(2*(R)*i-i*i); //y coordinate at x=R-i
        int y2=sqrt(2*(R)*(i-1)-(i-1)*(i-1));// y coordinate at
        int y= y1-y2;// number of lines parallel to
        s=s+y*(R-i)*4; //same number of integer pairs in all f
       }
        T=(s+1+(4*R));// total number of integer pairs
       printf("  N[%d]=",R);
       printf("%d",T);
       }
}

 N[1]=5  N[2]=13  N[3]=29  N[4]=49  N[5]=81  N[6]=113  N[7]=149  N[8]=1
529  N[14]=613  N[15]=709
```

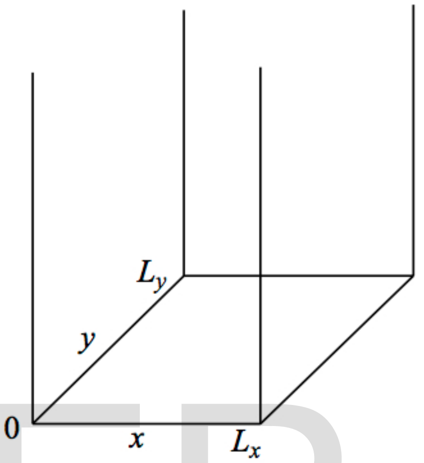
Particle in the box problem:

In quantum mechanics, the particle in a box model (also known as the infinite potential well or the infinite square well) describes a particle free to move in a small space surrounded by impenetrable barriers[3]

Suppose a x-y plane where the presence of potential is given by

$v(x,y) = 0$ for $(0 < x < L_x)$ and $(0 < y < L_y)$.

$v(x,y) = \infty$ otherwise



Where, $v(x,y)$ is the potential which is function of space. As potential is infinite beyond the boundaries particle is constrained to move in the 2D box.

Time independent Schrodinger wave equation then becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2}+\frac{\partial^2\psi(x,y)}{\partial y^2}\right)=E\psi(x,y). \quad [2]$$

Again, we have an equation in which only one term is x-dependent, so it must be a constant (which we take to be negative for future convenience),

$$\frac{\frac{\partial^2 f(x)}{\partial x^2}}{f(x)}=-C,\text{ say, so }\frac{\partial^2 f(x)}{\partial x^2}=-Cf(x).$$

Also,

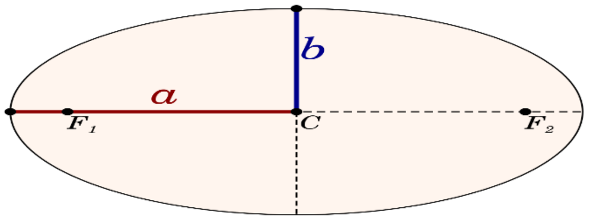
$$f(x)=A\sin\frac{n\pi x}{a}$$

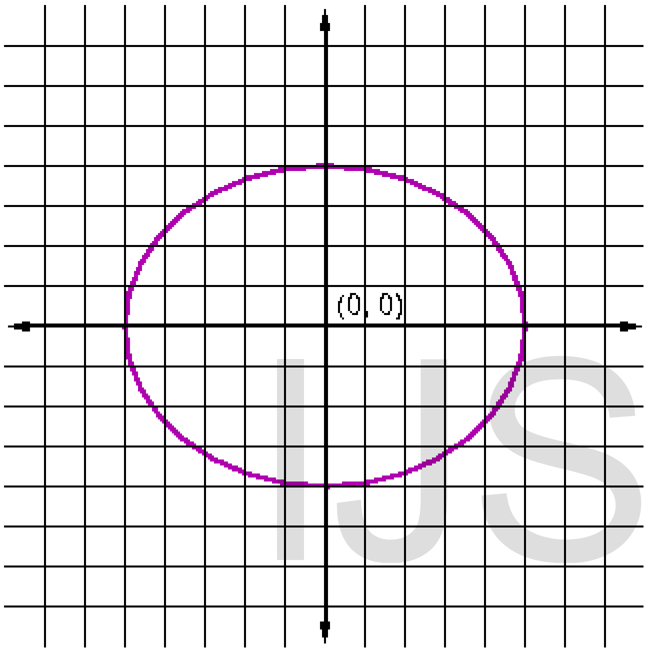
$$E_{n,m}=\frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2}+\frac{m^2\pi^2}{b^2}\right)$$

Where a and b are the length of the box on x-axis and y-axis and n and m are the corresponding energy levels respectively.

Hence energy is quantized

Here to find the number of states available to a particle we consider an ellipse instead of circle as length of both coordinates might be not same rest following the same algorithm will give us the desired result, where we have to calculate the number of intersections of lines.





Therefore for energy

$$E = R\frac{\hbar^2 \cdot \pi^2}{2m}$$

Where R is the energy level now,

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = R$$

Therefore

$$y = b \cdot \left(\sqrt{R - \frac{x^2}{a^2}}\right)$$

And the following the same algorithm but replacing circle by an ellipse we can evaluate the number of integer pairs and hence the quantum states available below a certain energy level.

Conclusion: This research demonstrates the algorithm to solve gauss circle problem. Here on every unit distance from origin on x and y axis perpendicular lines were drawn. Intersection of these lines occurred when both x and y coordinates were integer and hence by calculating the number of intersections we solved the gauss circle problem with integer Radius. This algorithm can be modified and applied to the a case where R is not an integer. Furthermore quantum states available for a certain energy level can be calculated by using a modified version of the equation where a circle in the gauss circle problem is to be replaced by an ellipse as dimensions of x-axis and y-axis allowed for the particle might not be same.

References:

1. https://en.wikipedia.org/wiki/Gauss_circle_problem
2. http://www.mecheng.iisc.ernet.in/~bobji/mspc/pdf/2d_wells.pdf
3. https://en.wikipedia.org/wiki/Particle_in_a_box