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USING MAPLE, MATHCAD SOFTWARE , METHODOLOGY FOR CREATING A PROGRAM SEQUENCE FOR DETERMINING THE SOLUTION OF THE STATIONARY SCHROEDENGER EQUATION IN DIFFERENT QUANTUM SYSTEMS.

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Below we will see how the **Maple system** solves some selected problems from quantum mechanics . In this case, we see the modeling of the problem in order to facilitate its further analysis and understanding. First, we analyze the solution of the stationary Schrödenger equation for a freely moving particle. In this case, the potential energy of the particle is zero. Thus, we introduce the following program and obtain the solution of the stationary Schrödenger equation [1]:

. > **# Free**

> **restart;**

> **U:=(x)->0;**

$$U := 0$$

> **a:=1;**

$$a := 1$$

> **schr:=diff(psi(x),x,x)+2*m/h^2*(EU(x))*psi(x)=0;**

$$schr := \left(\frac{\partial^2}{\partial x^2}\psi(x)\right) + \frac{2\,m\,E\,\psi(x)}{h^2} = 0$$

> **dsolve(schr);**

$$\psi(x) = \_C1\sin\left(\frac{\sqrt{2}\,\sqrt{m}\,\sqrt{E}\,x}{h}\right) + \_C2\cos\left(\frac{\sqrt{2}\,\sqrt{m}\,\sqrt{E}\,x}{h}\right)$$

Let's consider standing waves . Let's determine the solution of the noted stationary Schrödenger equation and analyze it. Between the walls, the particle potential energy is zero, because between the walls the particle forms freely. Thus[5]:

> **dsolve(diff(psi(x),x,x)+k^2*psi(x)=0);**

$$\psi(x) = \_C1\sin(k\,x) + \_C2\cos(k\,x)$$

Given the boundary conditions, of course, it is possible to determine the range of values that the wave vector **k** can take. Let's examine the normalized wave functions:

> **psi1:=(a,n,x)->1/sqrt(a)*sin(Pi*2*n/2/a*x);**

$$\psi 1 := (a, n, x) \to \frac{\sin\left(\frac{\pi n x}{a}\right)}{\sqrt{a}}$$

> **psi2:=(a,n,x)->1/sqrt(a)*cos(Pi*(2*n-1)/2/a*x);**

$$\psi 2 := (a, n, x) \to \frac{\cos\left(\frac{1}{2} \frac{\pi (2n-1) x}{a}\right)}{\sqrt{a}}$$

It is not difficult to check that they are normalized:

> **int(psi1(a,n,x)^2,x=-a..a);**

$$-\frac{\cos(\pi n) \sin(\pi n) - \pi n}{\pi n}$$

> **int(psi2(a,n,x)^2,x=-a..a);**

$$-\frac{2 \cos(\pi n) \sin(\pi n) + \pi - 2 \pi n}{\pi (2n-1)}$$

Analytical expressions for these functions can be obtained:

> **for n0 from 1 to 3 do psi1(a,n0,x);psi2(a,n0,x) od;**

$$\frac{\sin\left(\frac{\pi x}{a}\right)}{\sqrt{a}}$$

$$\frac{\cos\left(\frac{1}{2} \frac{\pi x}{a}\right)}{\sqrt{a}}$$

$$\frac{\sin\left(2 \frac{\pi x}{a}\right)}{\sqrt{a}}$$

$$\frac{\cos\left(\frac{3}{2} \frac{\pi x}{a}\right)}{\sqrt{a}}$$

$$\frac{\sin\left(3 \frac{\pi x}{a}\right)}{\sqrt{a}}$$

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$$\frac{\cos\left(\frac{5}{2}\frac{\pi x}{a}\right)}{\sqrt{a}}$$

- for example, to determine the average value of the impulse (operator), it is necessary to perform an exact integration [2]:

> **int(u1(a,n,x)*diff(u1(a,n,x),x),x=-a..a);**

$$0$$

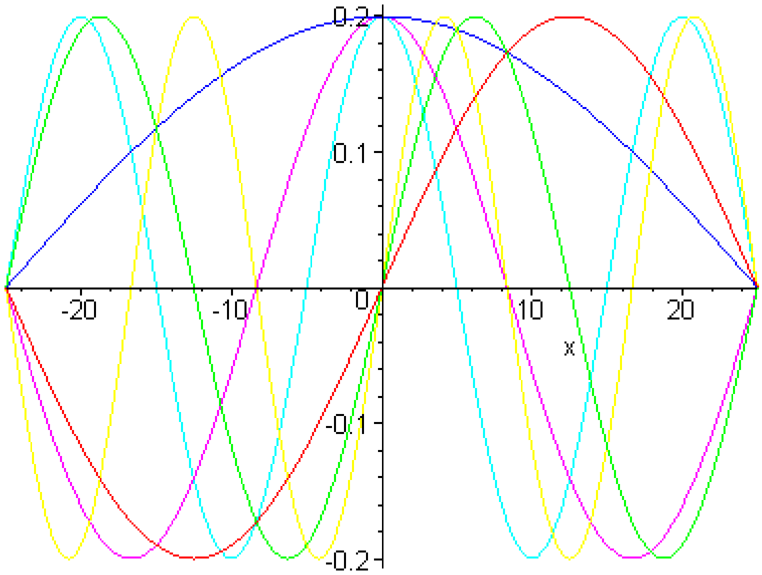
> **int(u1(a,n,x)*diff(u1(a,n,x),x),x=-a..a);**

$$0$$

It is also possible to construct the graphs of the first three (odd and even) eigenfunctions for the quantity a=25[3,4]:

> **plot([psi1(25,1,x),psi1(25,2,x),psi1(25,3,x),psi2(25,1,x),psi2(25,2,x),psi2(25,3,x)],x=-25..25);**

Let's examine the motion of a particle between two walls located at the points x=-a and x=a and completely impermeable to the particle. Let's say that at the point x=0 there is a very thin and very high (very high energy potential) barrier that half-transmits the de Broglie wave of the particle. In this case, let's analyze the solution of the Schrödenger equation, which describes the motion of the particle. It is known from the theoretical solutions of this problem that the statistical ensemble states of the considered system are represented by even and odd state functions [2]. - for example, it can be expressed as an odd state function $\psi_n^{(-)}(x) = \pm\sqrt{\frac{1}{a}}sin(\frac{\pi n x}{a} + \pi n), n = 1,2,3,\ldots$ Now let's create graphs of the first three state functions[5,6,7]:



Here we stop the information about the use of **Maple, MathCAD programs in solving physics problems, as well as in scientific research in this field.** Because if technology, especially nanoelectronics, develops in this way, there is no doubt that such problems will be easily solved in the near future.

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