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Cauchy & Fundamental Solutions of Linear Schrodinger PDEs

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Abstract **– Linear Schrodinger Partial Differential Equations (PDEs) are very important in applications including wave mechanics, quantum mechanics, particle physics, modern optics and much more found in physics, electrical engineering, and industrial applied mathematics. This article covers some practical examples and solutions of linear Schrodinger PDEs through definitions, then applications of it with corresponding examples and solutions. It is a basic equation in quantum mechanics where we solve for the wave function, Psi and where Planck's constant is h; mass is m; imaginary number is i ; and U(x) is the potential energy of the particle in the force field.**

Keywords **– Schrodinger, PDEs, Linear, Differential Equations, Evolution, Wave, Quantum**

I. Introduction

Linear Schrodinger Partial Differential Equations (PDEs) are very important in applications including wave mechanics, quantum mechanics, particle physics, modern optics and much more found in physics, electrical engineering, and industrial applied mathematics.

This article covers some practical examples and solutions of linear Schrodinger PDEs through definitions, then applications of it with corresponding examples and solutions.

It is a basic equation in quantum mechanics where we solve for the wave function, Psi and where Planck's constant is h; mass is m; imaginary number is i ; and U(x) is the potential energy of the particle in the force field.

II. Methodology and Motivation

The methodology or approach here involves using the books as cited in the References at the end of this article and separating the practical from the theory. There are actually very few, if any, practical examples of linear Schrodinger PDEs showing explicit general solutions, specifically Cauchy and Fundamental forms of these solutions in action out there in other journal articles.

III. Applications

Applications of linear Schrodinger PDEs include wave mechanics, quantum mechanics, particle physics, modern optics and much more found in physics, electrical engineering, and industrial applied mathematics.

Definition 3.1.

The wave function Psi (x, t) is continuous and belongs to a class C^2 of functions; hence this function is differentiable and smooth. Furthermore, U(x) is a potential energy of a particle in a force field. So, this one dimensional linear Schrodinger equation.

$$ih\Psi_t = -\frac{h^2}{2m}\Psi_{xx} + U(x)\Psi$$

will have a solution of the following form, where U(x) = 0, h is Planck's constant and m is the constant for mass.

$$\Psi(x,t) = exp(\frac{-iE_n}{h})U(x), U(x) = 0$$

Then, the solution of the Cauchy problem with the initial condition w = f(x) at t = 0 is given by the following:

$$\Psi(x,t) = \frac{1}{2\sqrt{i\pi\frac{ht}{2m}}}\int_{-\infty}^{\infty} exp[-\frac{(x-\xi)^2}{4\pi\frac{ht}{2m}}]f(\xi)d\xi$$

Source: W. Miller, Jr. (1977).

Remark 3.1.

Planck's constant h relates to the energy in one quantum (photon) in electromagnetic radiation to the frequency of that radiation. So, h ~ 6.626176 x 10-34 joule-seconds.

Example 3.1.

With the mass m = ½* pi or

$$m = \frac{\pi}{2}$$

The equation simplifies from the above definition and becomes this form:

$$ih\Psi_t = -\frac{h^2}{\pi}\Psi_{xx}$$

Therefore, the solution of the Cauchy problem with the initial condition w = f(x) at t = 0 is given by the following:

$$\Psi(x,t) = \frac{1}{2\sqrt{iht}}\int_{-\infty}^{\infty} exp[-\frac{(x-\xi)^2}{4ht}]f(\xi)d\xi$$

Definition 3.2.

The wave function Psi (x, t) is continuous and belongs to a class C^2 and U(x) be a potential energy of a particle in a force field, then there exists a solution of this equation.

$$ih\Psi_t = -\frac{h^2}{2m}\Psi_{xx} + U(x)\Psi$$

If U(x) = ax, then the above equations becomes the following:

$$ih\Psi_t = -\frac{h^2}{2m}\Psi_{xx} + ax\Psi$$

Then, the solution of the Cauchy problem with the initial condition w = f(x) at t = 0 is given by the following:

$$\Psi(x,t) = \frac{1}{2\sqrt{i\pi\frac{ht}{2m}}}exp[-\frac{i2amht}{h^2 2m}x - \frac{i}{3}(\frac{2am}{h^2})^2(\frac{2ht}{2m})^3]$$

$$* \int_{-\infty}^{\infty} exp[-\frac{(x+\frac{2am}{h^2}(\frac{ht}{2m})^2-\xi)^2}{4i\frac{ht}{2m}}]f(\xi)d\xi$$

Source: Miller, Jr. (1977).

Example 3.2.

With mass m = ½ and the constant a = 3, then the PDE in Definition 2 become the following:

$$a = 3, m = 1/2$$
$$ih\Psi_t = -h^2\Psi_{xx} + 3x\Psi$$

Then, using above definition, the solution of the Cauchy problem with the initial condition w = f(x) at t = 0 is given by the following:

$$\Psi(x,t) = \frac{1}{2\sqrt{i\pi ht}} exp[-i\frac{3tx}{h} - \frac{i}{3}(\frac{3}{h^2})^2(2ht)^3] * \int_{-\infty}^{\infty} exp[\frac{-(x+3t^2-\xi)^2}{4\pi ht}]f(\xi)d\xi$$

Definition 3.3.

The wave function Psi (x, t) is continuous and belongs to a class C^2 and U(x) be a potential energy of a particle in a force field, then there exists a solution of this equation:

$$i\Psi_t = \frac{-h^2}{2m}\Psi_{xx} + \frac{a}{x^2}\Psi$$

With U(x) = a/x^2 from above equation, then the wave function solution is of this form given the Cauchy problem with the initial condition w = f(x) at t = 0:

$$\Psi = \frac{exp[-\frac{1}{2}i\pi(\sqrt{\frac{2am}{h^2} + \frac{1}{4}} + 1)Sign(t)]}{2\left|\frac{ht}{2m}\right|} * \int_0^{\infty} \sqrt{xy} exp(i\frac{x^2+y^2}{4\frac{ht}{2m}}) * J_\mu(\frac{xy}{2\left|\frac{ht}{2m}\right|})f(y)dy$$

Source: W. Miller, Jr. (1977).

Example 3.3.

With mass m and a constant a having these values

$$a = \pi, m = \frac{h^2}{2}$$

Then, plugging in these values in above definition equation, we get the following simpler form of the equation:

$$ih\Psi_t = -\Psi_{xx} + \frac{\pi}{x^2}\Psi$$

Using these values, we get the following wave function solution given the Cauchy problem with the initial condition w = f(x) at t = 0:

$$\Psi = \frac{exp[-\frac{i\pi}{2}(\sqrt{\frac{\pi}{1} + \frac{1}{4}} + 1)Sign(t)]}{2\left|\frac{t}{h}\right|} * \int_0^{\infty} \sqrt{xy} exp(i\frac{x^2+y^2}{4\frac{t}{h}}) * J_\mu(\frac{xy}{2\left|\frac{t}{h}\right|})f(y)dy$$

Definition 3.4.

The wave function Psi (x, t) is continuous and belongs to a class C^2 where it is assumed the potential energy U(x) = 0. There exists a solution of this spatially two dimensional (2D) linear Schrodinger equation.

$$i\Psi_t + \frac{h^2}{2m}(\Psi_{xx} + \Psi_{yy}) = 0$$
$$\Psi_\varepsilon(x,y,t) = \frac{-im}{2\pi h^2 t} * exp[\frac{im}{2ht}(x^2+y^2) - i\frac{\pi}{2}]$$

Source: V.S. Vladimirov, V.P. Mikhailov, A.A. Varsharin, et al, . (1974).

Example 3.4.

With mass m having the following value:

$$m = \pi$$

And, plugging in this value to PDE in above definition, we get:

$$ih\Psi_t + \frac{h^2}{2\pi}(\Psi_{xx} + \Psi_{yy}) = 0$$

Where the fundamental solution is the following:

$$\Psi_\varepsilon(x,y,t) = \frac{-i}{2h^2t} * exp[\frac{i\pi}{2ht}(x^2+y^2) - i\frac{\pi}{2}]$$

Example 3.4.

With mass m having the following value

$$m = \pi h^2$$

And, plugging in this value to PDE in above definition, we get:

$$ih\Psi_t + \frac{h^2}{2\pi h^2}(\Psi_{xx} + \Psi_{yy}) = 0$$

Where the fundamental solution is the following:

$$\Psi_\varepsilon(x,y,t) = -\frac{i}{2t} exp[\frac{i\pi h}{2t}(x^2+y^2) - i\frac{\pi}{2}]$$

Definition 3.5.

The wave function Psi (x, t) is continuous and belongs to a class C^2 where it is assumed the potential energy U(x) = 0. There exists a solution of this spatially three dimensional (3D) linear Schrodinger equation.

$$i\Psi_t + \frac{h^2}{2m}(\Psi_{xx} + \Psi_{yy} + \Psi_{zz}) = 0$$
$$\Psi_\varepsilon(x,y,z,t) = -\frac{i}{h}(\frac{m}{2\pi ht})^{3/2} * exp[i\frac{m}{2ht}(x^2+y^2+z^2) - i\frac{3\pi}{4}]$$

Source: V.S. Vladimirov, V.P. Mikhailov, A.A. Varsharin, et al, . (1974).

Example 3.5.

With U(x) = 0 and mass of the following value

$$m = 2\pi h$$

Then, the PDE from above definition becomes the following:

$$ih\Psi_t + \frac{h^2}{4\pi h}(\Psi_{xx} + \Psi_{yy} + \Psi_{zz}) = 0$$

Where the fundamental solution becomes the following:

$$\Psi_\varepsilon(x,y,z,t) = -\frac{i}{h}(\frac{1}{t})^{3/2} * exp[\frac{\pi i}{t}(x^2+y^2+z^2) - i\frac{3\pi}{4}]$$

Example 3.5.

With the constant mass m = 6, then the PDE becomes the following:

$$ih\Psi_t + \frac{h^2}{12}(\Psi_{xx} + \Psi_{yy} + \Psi_{zz}) = 0$$

Therefore, from above definition, the fundamental solution is the following:

$$\Psi_\varepsilon(x,y,z,t) = \frac{-i}{h}(\frac{3}{\pi ht})^{3/2} * exp[\frac{3i}{ht}(x^2+y^2+z^2) - i\frac{3\pi}{4}]$$

Definition 3.6.

The wave function Psi (x, t) is continuous and belongs to a class C^2 where it is assumed the potential energy U(x) = 0. There exists a solution of this spatially n dimensional linear Schrodinger equation.

$$i h \Psi_t + \frac{h^2}{2m} \sum_{k=1}^{n} \Psi_{xx} = 0$$

With the following fundamental solution:

$$\Psi_\varepsilon(\boldsymbol{x}, t) = \frac{-i}{h} (\frac{m}{2\pi h t})^{n/2} * exp[i \frac{m}{2ht} |\boldsymbol{x}|^2 - i \frac{\pi n}{4}]$$

Source: V.S. Vladimirov, V.P. Mikhailov, A.A. Varsharin, et al, . (1974).

Example 3.6.

Using the above definition, apply n = 4 to make a 4th dimensional PDE below with mass m = 2:

This yields the following 4D Schrodinger PDE.

$$i h \Psi_t + \frac{h^2}{4} \sum_{k=1}^{4} \Psi_{xx} = 0$$

With the following fundamental solution for it.

$$\Psi_\varepsilon(\boldsymbol{x}, t) = \frac{-i}{h} (\frac{1}{\pi h t})^2 exp[\frac{i}{ht} |\boldsymbol{x}|^2 - i\pi]$$

Remark 3.2.

For 2D, 3D and nth dimensional linear Schrodinger PDEs above, if there were a non-zero form of potential energy U(x, y), U(x, y, z), etc., then Eigenvalues would need to be introduced, beyond the scope of this article.

IV. Conclusions

The solutions above are general solutions with Cauchy boundary conditions for 1D linear Schrodinger PDEs and Fundamental solutions for 2D, 3D and nth dimensional (space) linear Schrodinger PDEs.

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