On Laplace Transform Method for Schrӧdinger-like Equations

Bijon Biswas

Assistant Professor & HOD
Department of Mathematics,
P.K.H.N Mahavidyalaya, Howrah-711410, India

Abstract: **A novel approach is proposed in this article to deal with Schrӧdinger-like equations. The wave equations may not be handled with any other commonly used analytical technique. A generalized form of potential $V(r) = V_0 + \frac{V_1}{r} + \frac{V_2}{r^2}$ is used to illustrate the proposed method namely Laplace transform method (LTM) and usefulness of the technique.**

Introduction

The Schrӧdinger equation is used to describe the changes over time of a physical system in which quantum effects, such as wave-particle duality, are significant in quantum mechanics [1]. This equation is a mathematical formulation to investigate quantum mechanical systems. Its derivation was a significant landmark in developing the theory of quantum mechanics. The equation serves as a mathematical model of the movement of waves. It is in general a linear partial differential equation, describing the time-evolution of the system's wave function.

This equation is not the only way to analyze quantum mechanical systems and make predictions, as there are other quantum mechanical formulations available in literature such as Klein-Gordon equation, Dirac equation etc.

It is easy to study the Klein-Gordon equation as it looks like Schrӧdinger equation but the question arises for Dirac equation. To study the Dirac equation many scholars always convert the equations to Schrӧdinger -like equations [2-3].

After the conversion, the next challenge is to find the solutions to these equations. Many scholars have developed methods like Nikiforov-Uvarov method, asymptotic iteration method, supersymmetric and shape invariance method, etc.

Here I'm going to discuss on a powerful tool namely Laplace transform method to deal with Schrӧdinger -like equation. Without loss of generality, the general form of Schrӧdinger -like equation is given as follows:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + f(V,r,c)\right]\Psi(r,t) = i\hbar\frac{\partial}{\partial t}\Psi(r,t) \qquad (1)$$

where m is the particle's reduced mass, V is its potential energy, ∇^2 is the Laplacian (a differential operator) and Ψ is the wave function. This is a linear partial differential equation and the Laplace transform method can be used to solve it.

The rest of the article is presented as follows: the methodology of the technique is presented in Section 2. Application of the method with some examples is presented in Section 3 and finally a conclusion is reached in Section 4.

2. Methodology:

This section devoted to the discussion underpinning the methodology of the technique for solving (1). Before presentation of this methodology I will first present the definitions and some properties of Laplace transform related to the solution of Schrӧdinger-like equations.

Definition 1. The Laplace transform is a widely used integral transform with many applications in physics and engineering. The Laplace transform of the function f is defined as follows:

$$L\{f(x)\}(s) = \int_0^\infty e^{-sx} f(x)dx \qquad (2)$$

2.1 Some relevant Properties of Laplace transformation:

Suppose the differential equation contain a term of the form $t^m y^{(n)}(t)$ i.e., $t^m \frac{d^n y(t)}{dt^n}$. Then the Laplace transform of the term is represented by

$$L\left\{t^m \frac{d^n y(t)}{dt^n}\right\} = (-1)^m \frac{d^m}{ds^m} L\{y^{(n)}(t)\} \qquad (3)$$

So,

$$L\{ty''(t)\} = (-1)\frac{d}{ds}L\{y''(t)\} \qquad (4)$$

Again, another important theorem for Laplace transform of first order and second order derivative for continuous $y(t)$ and $y'(t)$ with $t \geq 0$ of exponential order σ as $t \to \infty$ and if $y'(t)$ and $y''(t)$ is of class A, then Laplace transform of $y'(t)$ and $y''(t)$ for $s > \sigma$ are given by

$$L\{y'(t)\} = sL\{y(t)\} - y(0) \quad (5)$$

And

$$L\{y''(t)\} = s^2L\{y(t)\} - sy(0) - y'(0) \quad (6)$$

One of the most important properties to be used in calculation is: if $y(t)$ is a function of class A, then

$$L\{t^n y(t)\} = (-1)^n \frac{d^n f(s)}{ds^n} \quad (7)$$

Where, $f(s) = L\{y(t)\} = \int_0^\infty y(t)e^{-ts}\,dt$ and $n = 1,2,3, \dots \dots \dots$

After conversion of second order differential equation to a first order one, we further apply the inverse Laplace transform to obtain the wave function. The relevant formulas for inverse Laplace transform are followed from [4].

3. Application on Dirac Equation:

3.1 Transformation of Dirac Equation to Schrödinger-like equation:

The Dirac equation of a nucleon with mass M moving in moving in an attractive scalar potential S(r) and a repulsive vector potential V (r) for spin-$\frac{1}{2}$ particles in the relativistic unit ($\hbar = c = 1$) is [5-8]

$$[\alpha.p + \beta(M + S(r))]\psi(r) = [E - V(r)]\psi(r) \quad (8)$$

where E is the relativistic energy of the system, $p = -i\nabla$ is the three dimensional momentum operator and M is the mass of the fermionic particle. α, β are the 4×4 Dirac matrices [8]. The eigenvalues of the spin-orbit coupling operator are $k = \left(j + \frac{1}{2}\right) > 0, k = -\left(j + \frac{1}{2}\right) < 0$ for the unaligned spin $j = l - \frac{1}{2}$ and aligned spin $j = l + \frac{1}{2}$ respectively. The set $(H; K; J^2; J_z)$ forms a complete set of conserved quantities. Using well-known identities,

$$(\sigma.A)(\sigma.B) = A.B + i\sigma.(A \times B),$$
$$\sigma.p = \sigma.\hat{r}\left(\hat{r}.p + i\frac{\sigma.L}{r}\right) \quad (9)$$

as well as the relations

$$(\sigma.L)Y_{jm}^{\tilde{l}}(\theta,\varphi) = (k-1)Y_{jm}^{\tilde{l}}(\theta,\varphi),$$
$$(\sigma.L)Y_{jm}^{l}(\theta,\varphi) = -(k+1)Y_{jm}^{l}(\theta,\varphi),$$
$$(\sigma.\hat{r})Y_{jm}^{l}(\theta,\varphi) = -Y_{jm}^{\tilde{l}}(\theta,\varphi),$$
$$(\sigma.\hat{r})Y_{jm}^{\tilde{l}}(\theta,\varphi) = -Y_{jm}^{l}(\theta,\varphi) \quad (10)$$

We find the following two coupled first-order Dirac equation,

$$\left(\frac{d}{dr} + \frac{k}{r}\right)F_{nk}(r) = \left(M + E_{nk} - \Delta(r)\right)G_{nk}(r) \quad (11)$$
$$\left(\frac{d}{dr} - \frac{k}{r}\right)G_{nk}(r) = \left(M - E_{nk} + \Sigma(r)\right)F_{nk}(r) \quad (12)$$

Where,

$$\Delta(r) = V(r) - S(r)$$
$$\Sigma(r) = V(r) + S(r)$$

One can easily obtain the second-order Schrödinger-like equation through elimination of $F_{nk}(r)$ and $G_{nk}(r)$ from above two equations

$$\left\{\frac{d^2}{dr^2} - \frac{k(k+1)}{r^2} - \left(M + E_{nk} - \Delta(r)\right)\left(M - E_{nk} + \Sigma(r)\right) + \frac{\frac{d\Delta(r)}{dr}\left(\frac{d}{dr} + \frac{k}{r}\right)}{\left(M + E_{nk} - \Delta(r)\right)}\right\}F_{nk}(r) = 0 \quad (13)$$

$$\left\{\frac{d^2}{dr^2} - \frac{k(k-1)}{r^2} - \left(M + E_{nk} - \Delta(r)\right)\left(M - E_{nk} + \Sigma(r)\right) + \frac{\frac{d\Sigma(r)}{dr}\left(\frac{d}{dr} - \frac{k}{r}\right)}{\left(M - E_{nk} + \Sigma(r)\right)}\right\}G_{nk}(r) = 0 \quad (14)$$

Where, $k(k+1) = l(l+1)$ and $k(k-1) = \bar{l}(\bar{l}+1)$.

We consider bound state solutions that demand the radial components satisfying $F_{nk}(0) = G_{nk}(0) = 0$ and $F_{nk}(\infty) = G_{nk}(\infty) = 0$.

3.2 Bound State Solutions for spin symmetry:

In the case of exact spin symmetry $\frac{d\Delta(r)}{dr} = 0$, i.e., $\Delta(r) = C = const$, Eq.(13) becomes

$$\left\{\frac{d^2}{dr^2} - \frac{k(k+1)}{r^2} - \left(M + E_{nk} - \Delta(r)\right)\left(M - E_{nk} + \Sigma(r)\right)\right\}F_{nk}(r) = 0 \quad (15)$$

Where, $k = l$ for $k < 0$ and $k = -(l+1)$ for $k > 0$. The energy eigenvalues depend on n and l, i.e., $E_{nk} = E(n; l(l+1))$, which is well known as the exact spin symmetry. We assume that $\Sigma(r) = V(r)$ and the Eq. (15) takes the form with this potential is :

$$\left\{\frac{d^2}{dr^2}-\frac{k(k+1)}{r^2}-(M+E_{nk}-C)\left(M-E_{nk}+V_0+\frac{V_1}{r}+\frac{V_2}{r^2}\right)\right\}F_{nk}(r)=0 \qquad (16)$$

Now defining the function $F_{nk}(r)=\sqrt{r}\varphi(r)$, we get

$$\left\{r^2\frac{d^2}{dr^2}+r\frac{d}{dr}-(\lambda^2r^2+\mu^2r+\nu^2)\right\}\varphi(r)=0 \qquad (17)$$

Where,

$$\lambda^2=(M+E_{nk}-C)(M-E_{nk}+V_0);\ \mu^2=\frac{1}{4}+V_1(M+E_{nk}-C);$$
$$\nu^2=k(k+1)+V_2(M+E_{nk}-C) \qquad (18)$$

Setting $\varphi(r)=r^{\beta}\emptyset(r)$, where β is a constant. Then equation (17) reduces to

$$\left\{r^2\frac{d^2}{dr^2}+(2\beta+1)r\frac{d}{dr}-(\lambda^2r^2+\mu^2r+\nu^2-\beta^2)\right\}\emptyset(r)=0 \qquad (19)$$

In order to obtain a finite wave function when $r\to\infty$, we must take $\beta=-\nu$ in equation (19) and then we get

$$\left\{r\frac{d^2}{dr^2}-(2\nu-1)\frac{d}{dr}-\lambda^2r-\mu^2\right\}\emptyset(r)=0 \qquad (20)$$

This form of equation is suitable for the application of LTM which is described above in section 2.1 and applying the LTM to the above equation we obtain a first order differential equation

$$(t^2-\lambda^2)\frac{df(t)}{dt}+[(2\nu+1)t+\mu^2]f(t)=0 \qquad (21)$$

Where $f(t)=L\{\emptyset(r)\}$ and the solution is given by

$$f(t)=N(t+\lambda)^{-(2\nu+1)}\left(\frac{t-\lambda}{t+\lambda}\right)^{-\frac{\mu^2}{2\lambda}-\frac{2\nu+1}{2}} \qquad (22)$$

The wave functions required to be single-valued but the term $\left(\frac{t-\lambda}{t+\lambda}\right)^{-\frac{\mu^2}{2\lambda}-\frac{2\nu+1}{2}}$ is multi-valued. Therefore, we must have to take

$$-\frac{\mu^2}{2\lambda}-\frac{2\nu+1}{2}=n,(n=0,1,2,\dots\dots\dots) \qquad (23)$$

Now applying a simple series expansion to equation (22) we obtain

$$f(t)=N'\sum_{m=0}^{n}\frac{(-1)^m n!}{(n-m)!\,m!}(2\lambda)^m(t+\lambda)^{-(2\nu+1)-m} \qquad (24)$$

Where N' is a constant. Using the inverse Laplace transformation in equation (24), we get

$$\emptyset(r)=N''r^{2\nu}e^{-\lambda r}\sum_{m=0}^{n}\frac{(-1)^m n!}{(n-m)!\,m!}\frac{\Gamma(2\nu+1)}{\Gamma(2\nu+1+m)}(2\lambda r)^m$$
$$=N''r^{2\nu}e^{-\lambda r}\ {}_1F_1(-n;2\nu+1;2\lambda r) \qquad (25)$$

Where ${}_1F_1(-n;2\nu+1;2\lambda r)$ is the notation of confluent hypergeometric function[9]. We also obtain

$$\varphi(r)=N'''r^{\nu}e^{-\lambda r}\ {}_1F_1(-n;2\nu+1;2\lambda r) \qquad (26)$$

Finally, we obtain the upper component of the Dirac spinor is obtained as

$$F_{nk}(r)=Nr^{\nu+\frac{1}{2}}e^{-\lambda r}\ {}_1F_1(-n;2\nu+1;2\lambda r) \qquad (27)$$

Where N is the normalization constant.

In order to find the lower component spinor, the recurrence relation of the confluent hypergeometric function

$$\frac{d}{dr}\ {}_1F_1(a;b;r)=\frac{a}{b}\ {}_1F_1(a+1;b+1;r) \qquad (28)$$

is used to evaluate equation (11) and this is obtained for spin symmetry case (i.e. for $\Delta(r)=C=const$) as

$$G_{nk}(r)=\frac{Nr^{\nu+\frac{1}{2}}e^{-\lambda r}}{M+E_{nk}-C}\left\{\frac{-n}{2\lambda(2\nu+1)}\ {}_1F_1(-n+1;2(\nu+1);2\lambda r)+\left(\frac{k+\nu+\frac{1}{2}}{r}-\lambda\right)\ {}_1F_1(-n;2\nu+1;2\lambda r)\right\} \qquad (29)$$

Using the equations (18) and (23), an explicit expression for the energy eigenvalues of the Dirac equation with $V(r)$ under the spin symmetry condition is obtained as:

$$-V_1\tilde{E}_{nk}=\frac{1}{4}+\left\{1+2n+2\sqrt{k(k+1)+V_2\tilde{E}_{nk}}\right\}\sqrt{\tilde{E}_{nk}(2M+V_0-C-\tilde{E}_{nk})} \qquad (30)$$

Where, $\tilde{E}_{nk}=M+E_{nk}-C$.

3.3 Bound State Solutions for pseudo-spin symmetry:

In the case of exact pseudo-spin symmetry $\frac{d\sum(r)}{dr}=0$, i.e., $\sum(r)=C_{ps}=const$, Eq. (14) becomes

$$\left\{\frac{d^2}{dr^2}-\frac{k(k-1)}{r^2}-\big(M+E_{nk}-\Delta(r)\big)\big(M-E_{nk}+C_{ps}\big)\right\}G_{nk}(r)=0 \qquad (31)$$

Where, k is related to the pseudo-orbital angular quantum number $\bar{l}$ as $k(k-1)=\bar{l}(\bar{l}+1)$, $k=-\bar{l}$ for $k<0$ and $k=(\bar{l}+1)$ for $k>0$, which implies that $j=\bar{l}\pm\frac{1}{2}$ are degenerate for $\bar{l}\neq 0$. It is required that the upper and lower spinor components must satisfy the following boundary conditions $F_{nk}(0)=G_{nk}(0)=0$ and $F_{nk}(\infty)=G_{nk}(\infty)=0$ for bound state solutions. The energy eigenvalues depend on n and $\bar{l}$, i.e., $E_{nk}=E\left(n,\bar{l}(\bar{l}+1)\right)$, which is well known as the exact spin symmetry. We assume that $\Delta(r)=V(r)$ and the Eq. (31) takes the form with this form of potential is :

$$\left\{\frac{d^2}{dr^2}-\frac{\bar{l}(\bar{l}+1)}{r^2}-\left(M+E_{nk}-V_0-\frac{V_1}{r}-\frac{V_2}{r^2}\right)\left(M-E_{nk}+C_{ps}\right)\right\}G_{nk}(r)=0 \qquad (32)$$

Now applying same procedure as above by defining the function $G_{nk}(r)=\sqrt{r}\varphi(r)$, we get

$$\left\{r^2\frac{d^2}{dr^2}+r\frac{d}{dr}-(\lambda^2r^2+\mu^2r+\nu^2)\right\}\varphi(r)=0 \qquad (33)$$

Where,

$$\lambda^2=\tilde{E}\left(2M-\tilde{E}+C_{ps}-V_0\right);\ \mu^2=V_1\tilde{E};$$
$$\nu^2=\bar{l}(\bar{l}+1)-V_2\tilde{E} \qquad (34)$$

Where, we assume $\tilde{E}=M-E+C_{ps}$.

Equation (33) is similar to equation (17) and so, via the calculations like the above one, the lower component of the Dirac spinor can be obtained as

$$G_{nk}(r)=\tilde{N}r^{\nu+\frac{1}{2}}e^{-\lambda r}\ {}_1F_1(-n;2\nu+1;2\lambda r) \qquad (35)$$

Where $\tilde{N}$ is the normalization constant and ${}_1F_1(-n;2\nu+1;2\lambda r)$ is the notation of confluent hypergeometric function.

In order to find the upper component spinor, the recurrence relation of the conuent hypergeometric function

$$\frac{d}{dr}\ {}_1F_1(a;b;r)=\frac{a}{b}\ {}_1F_1(a+1;b+1;r) \qquad (36)$$

is used to evaluate equation (12) and this is obtained for pseudo-spin symmetry case (i.e. for $\sum(r)=C_{ps}=const$) as

$$F_{nk}(r)=\frac{\tilde{N}r^{\nu+\frac{1}{2}}e^{-\lambda r}}{\tilde{E}}\left\{\frac{-n}{2\lambda(2\nu+1)}\ {}_1F_1(-n+1;2(\nu+1);2\lambda r)+\left(\frac{\nu+\frac{1}{2}-k}{r}-\lambda\right)\ {}_1F_1(-n;2\nu+1;2\lambda r)\right\} \qquad (37)$$

Where, $\tilde{N}$ is the normalization constant.

Also, in the similar fashion as obtained in the case of the spin symmetry condition, an explicit expression for the energy eigenvalues of the Dirac equation with $V(r)$ under the pseudo-spin symmetry is obtained as:

$$-V_1\tilde{E}=\frac{1}{4}+\left\{1+2n+2\sqrt{\bar{l}(\bar{l}+1)-V_2\tilde{E}}\right\}\sqrt{\tilde{E}(2M-\tilde{E}+C_{ps}-V_0)} \qquad (38)$$

Where, $\tilde{E}=M-E+C_{ps}$ and $k(k-1)=\bar{l}(\bar{l}+1)$.

Conclusion

It is important to point out that solving an equation analytically and finding the exact solution are more than proving the existence of the solution. For equations dealing with real world problems instead focus on developing methods to find analytical solutions of these equations since we need them to predict the behaviour of these physical phenomena. Numerical methods can also be used for this purpose. The main aim of this article is to propose a method that can be used to solve Schrödinger-like equations that other commonly used methods, such as the Nikiforov-Uvarov method, the reduced differential method, the shifted $\frac{1}{N}$ method, as well as the recent developed iteration methods, cannot handle. I therefore presented an example on Dirac equation which is not directly look like Schrödinger equation. The method proposed here makes use of the Laplace transform.

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