Our New Relativistic Wave Equation and Hydrogen-Like Atoms

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Abstract

In this paper, we look further into one of the relativistic wave equations we have introduced recently. Our relativistic wave equation is a PDE that is rooted in the relativistic energy Compton momentum relation, rather than the standard energy momentum relation. They are two sides of the same coin, but the standard momentum is just a derivative of the Compton momentum, so this simplifies things considerably. Here the main focus is to rewrite our relativistic PDE wave equation in spherical polar coordinates, then by some separation of variables we end up with three ordinary differential equations (ODEs) for which we present possible solutions, and we also provide a table where we compare our ODEs with the ODEs one gets from the Schrödinger equation [1]. This approach is used to describe hydrogen-like atoms. We encourage other researchers to check our calculations and the predictions from our solutions and see how they fit compared to observations from hydrogen-like atoms.

Key Words: quantum mechanics, Haug equation, Schrödinger equation, polar coordinates, ODEs, hydrogen-like atoms.

1 Solving Our New Relativistic Wave Equation for Hydrogen-like Atoms

The Haug-1 wave-equation [2] is given by

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-ci\hbar\nabla + V\right)\psi \tag{1}$$

where V is the potential energy, and $-i\hbar\nabla$ is the Compton momentum operator. The potential energy between two charges can easily be described by the Coulomb force [3]

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} = -k_e\frac{Ze^2}{r}$$

where k_e is Coulomb's constant. Further, our wave equation rewritten in polar coordinates is given by

$$E\psi = \left(-i\hbar c\left(\frac{\partial}{\partial r} + \frac{1}{r}\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\right) + V\right)\psi \tag{2}$$

where θ is the polar angle, with φ for the azimuthal angle, and $\psi = \psi(r,\theta,\phi)$.

The hydrogen atom's Hamiltonian is

$$\hat{H} = -i\hbar c\nabla - k_e\frac{Ze^2}{r} \tag{3}$$

where $-i\hbar\nabla$ is a Compton momentum operator.

The Haug relativistic wave equation for the hydrogen atom in polar coordinates is given by

$$E\psi = \left(-i\hbar c\left(\frac{\partial}{\partial r} + \frac{1}{r}\frac{\partial}{\partial\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\right) - \frac{Ze^2}{4\pi\epsilon_0 r}\right)\psi \tag{4}$$

This we can rearrange as

$$\frac{i}{\hbar c}\left(E + \frac{Ze^2}{4\pi\epsilon_0 r}\right)\psi = -\frac{\partial\psi}{\partial r} - \frac{1}{r}\frac{\partial\psi}{\partial\theta} - \frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi} \tag{5}$$

Next we rely on separation of variables

$$\psi(r,\theta,\phi) = R(r)\cdot Y(\theta,\phi) \tag{6}$$

Further, since Y does not depend on r, we can move it in front of the radial derivative, which gives

$$\frac{\partial\psi}{\partial r} = \frac{\partial}{\partial r}RY = Y\frac{dR}{dr} \tag{7}$$

and we therefore have

$$\frac{i}{\hbar c}\left(E - \frac{Ze^2}{4\pi\epsilon_0 r}\right)RY = Y\frac{dR}{dr} + R\frac{1}{r}\frac{\partial Y}{\partial\theta} + \frac{R}{r\sin\theta}\frac{\partial Y}{\partial\varphi} \tag{8}$$

Next we multiply by r and divide by RY to separate the radial and angular terms:

$$\frac{r}{R}\frac{dR}{dr} + \frac{1}{Y}\frac{\partial Y}{\partial\theta} + \frac{1}{Y\sin\theta}\frac{\partial Y}{\partial\varphi} - \frac{ir}{\hbar c}\left(E - \frac{Ze^2}{4\pi\epsilon_0 r}\right) = 0 \tag{9}$$

The first and last terms only depend on r, while the two middle terms depend on the angle. We can therefore separate the equation into two ordinary ODEs. We get a radial equation that is a first order ODE:

$$\frac{r}{R}\frac{dR}{dr} - \frac{ir}{\hbar c}\left(E - \frac{Ze^2}{4\pi\epsilon_0 r}\right) - A = 0 \tag{10}$$

where the solution is

$$R(r) = c_1 e^{\frac{\log(r)\left(Ac\hbar + izk_e e^2\right) - iEr}{c\hbar}} \tag{11}$$

where A must likely be a positive integer as energy comes as $n\hbar$. And we also get a first order PDE linked to the angles:

$$\begin{aligned}\frac{1}{Y}\frac{\partial Y}{\partial\theta} + \frac{1}{Y\sin\theta}\frac{\partial Y}{\partial\varphi} + A &= 0\\ \frac{\partial Y}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial Y}{\partial\varphi} + AY &= 0\end{aligned} \tag{12}$$

where A is a separation constant.

Still, the angle equation still contains terms for both φ and θ, so we need to do one more separation of variables:

$$Y(\theta,\phi) = \Theta(\theta)\cdot\Phi(\phi) \tag{13}$$

Replacing Y in the differential equation, we get

$$\Phi\frac{d\Theta}{d\theta} + \frac{\Theta}{\sin\theta}\frac{d\Phi}{d\varphi} + A\Theta\Phi = 0 \tag{14}$$

Next we isolate variables and separate terms

$$\Phi\frac{d\Theta}{d\theta} + \frac{\Theta}{\sin\theta}\frac{d\Phi}{d\varphi} + A\Theta\Phi = 0 \tag{15}$$

Next we divide by $\Theta\Phi$ to separate the radial and angular terms:

$$\frac{\sin\theta}{\Theta}\frac{d\Theta}{d\theta} + \frac{1}{\Phi}\frac{d\Phi}{d\varphi} + A\sin\theta = 0 \tag{16}$$

This we can separate into two new equations, the polar equation (colatitude)

$$\frac{\sin\theta}{\Theta}\frac{d\Theta}{d\theta} + A\sin\theta - B = 0 \tag{17}$$

and the azimuthal equation

$$\frac{1}{\Phi}\frac{d\Phi}{d\varphi}+B=0 \tag{18}$$

The given azimuthal equation has solution

$$\Phi(\phi)=c_1 e^{-B\phi} \tag{19}$$

The solution must be a valid solution for any angle ϕ, this means we must have

$$\Phi(\phi)=e^{-B2\pi}=e^{-B\times 0}=e^{-B\phi} \tag{20}$$

This mean B must be a positive integer for this to hold true, and B can therefore be seen as the Azimuthal quantum number.

For comparison, the Schrödinger Azimuthal ODE, $\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}+B=0$ has solution $\Phi(\phi)=c_1\cos\sqrt{B}\phi+c_2\sin\sqrt{B}\phi$, and when setting $c_1=1$ and $c_2=i$ is equal to $\Phi(\phi)=e^{i\sqrt{B}\phi}$. In the Schrödinger solution one do a trick that we need to think more about the validity of, one are here replacing B with m^2, and thereby get $\Phi(\phi)=e^{im\phi}$ which is basically is identical to our solution if we replace i with -1. But again to get to this solution from the Schrödinger equation one have to replace the constant B with m^2, and where did this come from mathematically? It possibly seems to be guess work that is a fudge to fit observations (if we are wrong on this we are happy to hear about a better explanation). In the solution to our Azimuthal ODE, then B itself is a quantum number, but in the Schrödinger solution one have to do this ad-hock assumption of setting $B=m^2$.

Further, our polar equation is given by

$$\frac{\sin\theta}{\Theta}\frac{d\Theta}{d\theta}+A\sin\theta-B \quad = \quad 0 \tag{21}$$

rearranging

$$\frac{1}{\Theta}\frac{d\Theta}{d\theta}+A-\frac{B}{\sin\theta} \quad = \quad 0 \tag{22}$$

and solving directly, using Mathematica gives

$$\Theta(\theta)=e^{-A\theta-B\log[\cos(\theta/2)]+B\log[\sin(\theta/2)]}c_1 \tag{23}$$

However, we can alternatively rewrite the polar equation somewhat before we solve it. Substituting $P(\cos\theta):=\Theta(\theta)$ and $x:=\cos\theta$, we get

$$\begin{aligned}\frac{-\sin\theta}{\Theta}\frac{dP}{dx}+A-\frac{B}{\sin\theta} &= 0\\ \frac{\sin\theta}{\Theta}\frac{dP}{dx}-A+\frac{B}{\sin\theta} &= 0\end{aligned} \tag{24}$$

since $\sin^2\theta+\cos^2\theta=1$, we have that, $\sin\theta=\sqrt{1-\cos^2\theta}$, and we can therefore rewrite the equation above as

$$\begin{aligned}\frac{\sin\theta}{P}\frac{dP}{dx}-A+\frac{B}{\sqrt{1-\cos^2\theta}} &= 0\\ \sqrt{1-x^2}\frac{dP}{dx}-\left(A+\frac{B}{\sqrt{1-x^2}}\right)P &= 0\end{aligned} \tag{25}$$

The coefficient in the ODE is not constant, but depends on x. One possible solution seems to be

$$P(x)=e^{A\arcsin[x]-B\,\mathrm{arctanh}[x]} \tag{26}$$

where A and B are positive integers, in other words quantum number, see further up for why.

For comparison with the Schrödinger equation, based on the same principles we get the following ODE

$$(1-x^2)\frac{d^2P}{dx^2}-2x\frac{dP}{dX}+\left(A+\frac{B}{1-x^2}\right)P=0 \tag{27}$$

The coefficients in the ODE we get from the Schrödinger equation are not constant, but depend on x. This is a differential equation known as a Legendre-type DE, with known solutions, still it is worth noticing it is much more complicated to solve than polar ODE from our new relativistic wave equation.

2 Our PDE Leads to Three ODEs

The radial equation

$$\frac{1}{R}\frac{dR}{dr}-\frac{i}{\hbar c}\left(E-k_e\frac{Ze^2}{r}\right)-\frac{AR}{r}=0 \tag{28}$$

Further, we have the azimuthal equation

$$\frac{1}{\Phi}\frac{d\Phi}{d\varphi}+B=0 \tag{29}$$

And the polar equation we get is

$$\frac{1}{\Theta}\frac{d\Theta}{d\theta}+A-\frac{B}{\sin\theta}=0 \tag{30}$$

compared to Schrödinger's polar equation for hydrogen-like atoms, which is given by $\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\frac{d\Theta}{d\theta}\right)+A-\frac{B}{\sin^2\theta}=0$.
Table 1 summarizes our findings and also makes it easy to compare to Schrödinger's equation.

Equations:	**Schrödinger :**	**Solution :**
Radial equation	$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2\mu r^2}{\hbar}\left(E-k_e\frac{Ze^2}{r}\right)R-AR=0$	$R_\infty=c_3e^{i\sqrt{\frac{2\mu E}{\hbar}}r}+c_4e^{-i\sqrt{\frac{2\mu E}{\hbar}}r}$
Azimuthal equation	$\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2}+B=0$	$\Phi(\phi)=e^{i\sqrt{B}\phi}$
Polar equation Rewritten	$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\frac{d\Theta}{d\theta}\right)+A-\frac{B}{\sin^2\theta}=0$ $(1\text{-x}^2)\frac{d^2P}{dx^2}-2x\frac{dP}{dX}+\left(A+\frac{B}{1-x^2}\right)P=0$	
Equations:	**From our new equation :**	**Solution :**
Radial equation	$\frac{r}{R}\frac{dR}{dr}-\frac{ir}{\hbar c}\left(E-zk_e\frac{Ze^2}{r}\right)-A=0$	$R(r)=c_1e^{\frac{\log(r)\left(Ac\hbar+izk_ee^2\right)-i\mathrm{E}r}{c\hbar}}$
Azimuthal equation	$\frac{1}{\Phi}\frac{d\Phi}{d\varphi}+B=0$	$\Phi(\phi)=c_1e^{-B\phi}$
Polar equation Rewritten	$\frac{1}{\Theta}\frac{d\Theta}{d\theta}+A-\frac{B}{\sin\theta}=0$ $\sqrt{1-x^2}\frac{dP}{dx}-\left(A+\frac{B}{\sqrt{1-x^2}}\right)P=0$	$\Theta(\theta)=c_1e^{-A\theta-B\log[\cos(\theta/2)]+B\log[\sin(\theta/2)]}$ $P(x)=e^{A\arcsin[x]-B\,\mathrm{arctanh}[x]}$

Table 1: The table shows three ODEs we get from the Schrödinger when written on polar coordinates, and also three ODEs we get from our new relativistic wave equation.

3 Conclusion

We have taken our new relativistic wave equation that is directly linked to the relativistic energy Compton momentum relation and put it into polar coordinate form. Next, by separation of variables this leads to three ODEs, which we can call the radial equation, the azimuthal equation, and the polar equation. We have also presented possible solutions for these ODEs. We encourage other researchers to check our solutions, and also to perform numerical calculations from our results and see if they fit observations for hydrogen-like atoms; we believe that these solutions should hold for such cases. Our three ODEs seem to be of a simpler form compared to what one gets from the Schrödinger equation. This is not a big surprise, as we claim that our PDE is linked more directly to the deeper aspects of the quantum world. Still, only further research can provide a final answer on whether or not this suggested path is useful. We will continue on this path and note that the proof will be in the pudding so to speak.

References

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