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 wav 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 polar coordinates, then by some separation of variables we end up with three ordinary differential equations (ODE's) for which we present solutions, and we also provide a table where we compare our ODE's with the ODE's one gets from the Schrödinger equation [1]. This approach is used to describe hydrogen-like atoms.

Key Words: quantum mechanics, de Broglie wavelength, Compton wavelength.

1 Solving for Hydrogen-like Atoms

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

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

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

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

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

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

where θ is the polar angle and φ for the azimuthal angle, and $\psi = \psi(r,\theta,\phi)$.
The hydrogen atom's Hamiltonian is

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

where $-i\hbar\nabla$ is a Compton momentum operator.
The Haug equation for the hydrogen atom in polar coordinates is given by

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

This we can rearrange as

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

Next we rely on separation of variables

$$\psi(r,\theta,\phi) = R(r)\cdot Y(\theta,\phi)$$

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

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

and we therefore have

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

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

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

The first and the last term 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:

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

and we get a first order PDE linked to the angles:

$$\begin{aligned}\frac{1}{Y}\frac{\partial Y}{\partial\theta} + \frac{1}{Y\sin\theta}\frac{\partial Y}{\partial\varphi} + A &= 0\\ \frac{\partial Y}{\partial\theta} + \frac{1}{\sin\theta}\frac{\partial Y}{\partial\varphi} + AY &= 0 \qquad (2)\end{aligned}$$

where A is a separation constant.

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

$$Y(\theta,\phi) = \Theta(\theta)\cdot\Phi(\phi)$$

Replacing Y in the differential equation we get

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

Next we isolate variables and separate terms

$$\Phi\frac{d\Theta}{d\theta} + \frac{\Theta}{\sin\theta}\frac{d\Phi}{d\varphi} + A\Theta\Phi = 0 \qquad (3)$$

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

$$\frac{\sin\theta}{\Theta}\frac{d\Theta}{d\theta} + \frac{1}{\Phi}\frac{d\Phi}{d\varphi} + A\sin\theta = 0 \qquad (4)$$

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

$$\frac{\sin\theta}{\Theta}\frac{d\Theta}{d\theta} + A\sin\theta - B = 0 \qquad (5)$$

and the azimuthal equation

$$\frac{1}{\Phi}\frac{d\Phi}{d\varphi} + B \quad = \quad 0 \tag{6}$$

gives solution

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

Schrödinger supposedly has a solution of $\Phi(\phi) = c_1 e^{i\sqrt{B}\phi} + c_2 e^{-i\sqrt{B}\phi}$. Further, our polar equation is given by

$$\frac{\sin\theta}{\Theta}\frac{d\Theta}{d\theta} + A\sin\theta - B \quad = \quad 0 \tag{7}$$

rearranging

$$\frac{1}{\Theta}\frac{d\Theta}{d\theta} + A - \frac{B}{\sin\theta} \quad = \quad 0 \tag{8}$$

and solving directly, using Mathematica gives

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

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

$$\begin{aligned} \frac{-\sin\theta}{\Theta}\frac{dP}{dx} + A - \frac{B}{\sin\theta} &= 0 \\ \frac{\sin\theta}{\Theta}\frac{dP}{dx} - A + \frac{B}{\sin\theta} &= 0 \end{aligned} \tag{9}$$

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

$$\begin{aligned} \frac{\sin\theta}{P}\frac{dP}{dx} - A + \frac{B}{\sqrt{1-\cos^2\theta}} &= 0 \\ \sqrt{1-x^2}\frac{dP}{dx} - \left(A + \frac{B}{\sqrt{1-x^2}}\right)P &= 0 \end{aligned} \tag{10}$$

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

$$P(x) = e^{A\arcsin[x] - B\,\mathrm{arctanh}[x]} \tag{11}$$

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

$$(1-x^2)\frac{d^2P}{dx^2} - 2x\frac{dP}{dX}\left(A + \frac{B}{1-x^2}\right)P \quad = \quad 0 \tag{12}$$

The coefficients in the ODE we get from the Schrödinger are not constant, but depends on x. This is a differential equation known as a Legendre-type DE, with known solutions.

2 Our PDE Leads to 3 ODEs

The radial equation

$$\frac{1}{R}\frac{dR}{dr} - \frac{i}{\hbar c}\left(E - k_e\frac{Ze^2}{r}\right) - \frac{AR}{r} = 0 \tag{13}$$

Further, we have the azimuth equation

$$\frac{1}{\Phi}\frac{d\Phi}{d\varphi} + B = 0 \tag{14}$$

And the polar equation we get is

$$\frac{1}{\Theta}\frac{d\Theta}{d\theta} + A - \frac{B}{\sin\theta} = 0 \tag{15}$$

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 Schrodinger.

Equations:	**Schrödinger :**	**Solution :**
Radial equation	$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2\mu r^2}{\hbar}\left(E - k_e\frac{Ze^2}{r}\right) - AR = 0$	$R_\infty = c_3 e^{i\sqrt{\frac{2\mu E}{\hbar}}r} + c_4 e^{-i\sqrt{\frac{2\mu E}{\hbar}}r}$
Azimuthal equation	$\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2} + B = 0$	$\Phi(\phi) = c_1 e^{i\sqrt{B}\phi} + c_2 e^{-i\sqrt{B}\phi}$
Polar equation Re-writen	$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\frac{d\Theta}{d\theta}\right) + A - \frac{B}{\sin^2\theta} = 0$ $(1\text{-x}^2)\frac{d^2P}{dx^2} - 2x\frac{dP}{dX} + \left(A + \frac{B}{1-x^2}\right)P = 0$	
Equations:	**From our new equation :**	**Solution :**
Radial equation	$\frac{r}{R}\frac{dR}{dr} - \frac{ir}{\hbar c}\left(E - k_e\frac{Ze^2}{r}\right) - AR = 0$	$R(r) \to \frac{r^{\frac{i\mathrm{E}}{c\hbar}}\left(\frac{ik_e e^2}{c\hbar r}\right)^{\frac{i\mathrm{E}}{c\hbar}} e^{\frac{i\left(-\frac{k_e e^2}{r} - \mathrm{E}\log(r)\right)}{c\hbar}}}{c_1 r^{\frac{i\mathrm{E}}{c\hbar}}\left(\frac{ik_e e^2}{c\hbar r}\right)^{\frac{i\mathrm{E}}{c\hbar}} - AGamma\left(\frac{i\mathrm{E}}{c\hbar}, \frac{ik_e e^2}{c\hbar r}\right)}$
	Rewritten solution:	$R(r) \to \frac{r^{\frac{i\mathrm{E}}{c\hbar}}\left(\frac{i\alpha}{r}\right)^{\frac{i\mathrm{E}}{c\hbar}} e^{i\left(-\frac{\alpha}{r} - \frac{\mathrm{E}\log(r)}{c\hbar}\right)}}{c_1 r^{\frac{i\mathrm{E}}{c\hbar}}\left(\frac{i\alpha}{r}\right)^{\frac{i\mathrm{E}}{c\hbar}} - AGamma\left(\frac{i\mathrm{E}}{c\hbar}, \frac{i\alpha}{r}\right)}$
Azimuthal equation	$\frac{1}{\Phi}\frac{d\Phi}{d\varphi} + B = 0$	$\Phi(\phi) = c_1 e^{-B\phi}$
Polar equation Re-written	$\frac{1}{\Theta}\frac{d\Theta}{d\theta} + A - \frac{B}{\sin\theta} = 0$ $\sqrt{1-x^2}\frac{dP}{dx} - \left(A + \frac{B}{\sqrt{1-x^2}}\right)P = 0$	$\Theta(\theta) = c_1 e^{-A\theta - B\log[\cos(\theta/2)] + B\log[\sin(\theta/2)]}$ $e^{A\arcsin[x] - B\,\mathrm{arctanh}[x]}$

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

References

[1] E. Schrödinger. An undulatory theory of the mechanics of atoms and molecules. *Physical Review*, 28(6): 104–1070, 1926.

[2] E. G. Haug. Deeper insight on existing and new wave equations in quantum mechanics. *ViXrA or Research-gate, submitted for review in a journal*, 2020. URL https://vixra.org/abs/2008.0010.