Quantum 1 Midterm, Klein-Gordon equation

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1 Klein-Gordon equation

We wish to determine the relativistic energy levels of hydrogen-like atoms. We consider the relativistic energy of a free particle:

$$E^2 = (mc^2)^2 + (pc)^2 \tag{1.1}$$
$$(pc)^2 + (mc^2)^2 - E^2 = 0 \tag{1.2}$$

We can convert this to a second-order PDE by using Schrodinger's substitution $p \rightarrow \frac{\hbar}{i}\nabla$. We now have a second-order operator acting on a wavefunction ψ:

$$\{(\frac{\hbar c}{i}\nabla)^2 + (mc^2)^2 - E^2\}\psi = 0 \tag{1.3}$$

We now put our free particle in a scalar potential V. This will be the electrostatic potential from the nuclear charge. Going back to 1.1, we substitute $(E - V)$ for E. The negative sign retains conservation of potential/kinetic energy (as potential energy goes up, the kinetic energy goes down).

$$\{(\frac{\hbar c}{i}\nabla)^2 + (mc^2)^2 - (E - V)^2)\}\psi = 0 \tag{1.4}$$
$$-(\hbar c)^2\nabla^2\psi + \{(mc^2)^2 - (E - V)^2\}\psi = 0 \tag{1.5}$$

The Laplacian in three dimensions is:

$$\nabla^2\chi(r, \phi, \theta) = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\chi}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\chi}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\chi}{\partial\phi^2} \tag{1.6}$$

We assume we can separate 1.5 into $\psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$. We can then use 1.6 to write 1.5 as:

$$\begin{aligned} -(\hbar c)^2\{\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{dR}{dr})\Phi\Theta + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{d\Theta}{d\theta})R\Phi \\ + \frac{1}{r^2\sin^2\theta}\frac{d^2\Phi}{d\phi^2}R\Theta\} + \{(mc^2)^2 - (E - V(r))^2\}R\Phi\Theta = 0 \end{aligned} \tag{1.7}$$

Dividing through by $\frac{-(\hbar c)^2 R\Theta\Phi}{r^2}$ we have:

$$\frac{1}{R}\frac{d}{dr}(r^2\frac{dR}{dr}) + \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta}) + \frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\phi^2} - r^2\frac{(mc^2)^2 - (E - V(r))^2}{(\hbar c)^2} = 0 \tag{1.8}$$

The first and fourth terms are expressions in r only, the second and third terms are expressions in θ and ϕ. We can therefore separate the angular and radial terms. The solutions to the angular terms are the spherical harmonics $P_\ell^m(\cos\theta)e^{im\phi}$. We examine the radial solution by setting the separation constant to $\ell(\ell+1)$, and we have:

$$\frac{1}{R}\frac{d}{dr}(r^2\frac{dR}{dr}) - r^2\frac{(mc^2)^2-(E-V(r))^2}{(\hbar c)^2} = \ell(\ell+1) \tag{1.9}$$

$$\frac{d}{dr}(r^2\frac{dR}{dr}) + \frac{Rr^2}{(\hbar c)^2}\{(E-V(r))^2-(mc^2)^2)\} - R(\ell(\ell+1)) = 0 \tag{1.10}$$

We make the substitution $R = \frac{u}{r}$. We then find:

$$R = \frac{u}{r} \tag{1.11}$$

$$\frac{dR}{dr} = \frac{u'}{r} - \frac{u}{r^2} = \frac{ru'-u}{r^2} \tag{1.12}$$

$$\frac{d}{dr}(r^2\frac{dR}{dr}) = \frac{d}{dr}(ru'-u) = ru'' \tag{1.13}$$

We can now substitute into 1.10:

$$r\frac{d^2u}{dr^2} + \frac{ur}{(\hbar c)^2}((E-V(r))^2-(mc^2)^2)) - \frac{u}{r}(\ell(\ell+1)) = 0 \tag{1.14}$$

$$\frac{d^2u}{dr^2} + \frac{u}{(\hbar c)^2}((E-V(r))^2-(mc^2)^2)) - \frac{u}{r^2}(\ell(\ell+1)) = 0 \tag{1.15}$$

We now introduce a dimensionless constant $r = \gamma z$ so that we can look up the solution for this PDE. This is also a good time to introduce our potential function, $V(r) = \frac{-e^2}{r}$.

$$\frac{1}{\gamma^2}\frac{d^2u}{dz^2} + \frac{u}{(\hbar c)^2}((E-\frac{-e^2}{\gamma z})^2-(mc^2)^2)) - \frac{u}{(\gamma z)^2}\ell(\ell+1) = 0 \tag{1.16}$$

$$\frac{1}{\gamma^2}\frac{d^2u}{dz^2} + \frac{u}{(\hbar c)^2}((E^2+2E\frac{e^2}{\gamma z}+(\frac{-e^2}{\gamma z})^2)-(mc^2)^2)) - \frac{u}{(\gamma z)^2}\ell(\ell+1) = 0 \tag{1.17}$$

$$\frac{d^2u}{dz^2} + \{\frac{1}{z}\frac{2Ee^2\gamma}{(\hbar c)^2} + \frac{-\ell(\ell+1)+\frac{e^4}{(\hbar c)^2})}{z^2} + \frac{\gamma^2}{(\hbar c)^2}(E^2-(mc^2)^2)\}u = 0 \tag{1.18}$$

We find a solution of the right form in Abramowitz and Stegun:

$$\frac{d^2y}{dx^2} + \{\frac{2n+\beta+1}{2x} + \frac{1-\beta^2}{4x^2} - \frac{1}{4}\}y = 0 \tag{1.19}$$

Equating terms and making the substitution $\alpha = \frac{e^2}{(\hbar c)^2}$, we find:

$$-\ell(\ell+1)+\alpha^2 = \frac{1-\beta^2}{4} \tag{1.20}$$

$$2E\alpha\frac{\gamma}{\hbar c} = \frac{2n+\beta+1}{2} \tag{1.21}$$

$$\frac{\gamma^2}{(\hbar c)^2}(E^2-(mc^2)^2) = -\frac{1}{4} \tag{1.22}$$

From the first equation we see that $4[(\ell+\frac{1}{2})^2-\alpha^2] = \beta^2$, so $\beta = 2\sqrt{(\ell+\frac{1}{2})^2-\alpha^2}$. We use the second equation to solve for $\frac{\gamma}{\hbar c}$, then plug into the third equation to find an expression for E.

$$2E\alpha\frac{\gamma}{\hbar c} = \frac{2n+\beta+1}{2} \tag{1.23}$$

$$2E\alpha\frac{\gamma}{\hbar c} = n+\sqrt{(\ell+\frac{1}{2})^2-\alpha^2}+\frac{1}{2},\ N(\alpha) \equiv n+\sqrt{(\ell+\frac{1}{2})^2-\alpha^2}+\frac{1}{2} \tag{1.24}$$

$$\frac{\gamma}{\hbar c} = \frac{N(\alpha)}{2E\alpha} \tag{1.25}$$

$$(\frac{N(\alpha)}{2E\alpha})^2(E^2-(mc^2)^2) = -\frac{1}{4} \tag{1.26}$$

$$-1+\frac{(mc^2)^2}{E^2} = (\frac{\alpha}{N(\alpha)})^2 \tag{1.27}$$

$$E^2 = \frac{(mc^2)^2}{1-(\frac{\alpha}{N(\alpha)})^2} \tag{1.28}$$

$$E = \frac{mc^2}{\sqrt{1-(\frac{\alpha}{N(\alpha)})^2}} \tag{1.29}$$

We can now substitute E into equation 1.21 to find γ.

$$2E\alpha\frac{\gamma}{\hbar c} = N(\alpha) \tag{1.30}$$

$$\gamma = \frac{\hbar c}{2mc^2}\sqrt{1-(\frac{\alpha}{N(\alpha)})^2}\frac{N(\alpha)}{\alpha} \tag{1.31}$$

$$\gamma = \frac{\hbar c}{2mc^2}\sqrt{(\frac{N(\alpha)}{\alpha})^2-1} \tag{1.32}$$

The presence of minus signs under square roots raises a question of imaginary values for the energy spectra. We examine the ground state, $n = \ell = 0$, so that $N(\alpha) = \frac{1}{2}+\sqrt{\frac{1}{4}-\alpha^2}$. Since the fine structure constant $\alpha \approx \frac{1}{137}$, this works fine for hydrogen. However it may fail for other atoms with a higher nuclear charge Ze (Z an integer). A nuclear charge of Ze will modify the expression for α to $\frac{(Ze)-e}{\hbar c} = Z\alpha$. We then find the nuclear charge at which $N(Z\alpha)$ becomes complex.

$$\frac{1}{4}-Z^2\alpha^2 = 0 \tag{1.33}$$

$$Z^2 = \frac{1}{4\alpha^2} \approx \frac{137^2}{2^2} \tag{1.34}$$

$$Z \approx \frac{137}{2} = 68.5 \tag{1.35}$$

So for nucleii with atomic number 69 (thulium) or greater the Klein-Gordon equation will produce complex numbers for the energy spectrum.
The rest energy mc^2 will typically dominate the total energy. Returning to equation 1.2, we expand $E = (mc^2+W)$ as the rest energy plus a nonrelativistic

energy W. We then expand $(E - V)^2$:

$$(mc^2 + W - V)^2 = (mc^2 + (W - V))^2 = (mc^2)^2 + 2mc^2(W - V) + (W - V)^2 \tag{1.36}$$

We then plug this into 1.2:

$$(pc)^2 + (mc^2)^2 - E^2 = 0 \tag{1.37}$$

$$(pc)^2 + (mc^2)^2 - \{(mc^2)^2 + 2mc^2(W - V) + (W - V)^2\} = 0 \tag{1.38}$$

$$(pc)^2 - 2mc^2(W - V) - (W - V)^2 = 0 \tag{1.39}$$

$$\frac{p^2}{2m} - (W - V) - \frac{(W - V)^2}{2mc^2} = 0 \tag{1.40}$$

In the nonrelativistic limit we can discard the third term and we recover the classical result (replacing W by E).

$$\frac{p^2}{2m} + V = E \tag{1.41}$$