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Saeed Mohammadi
Department of Physics, Payame Noor University, PO BOX 19395-3697 Tehran, Iran.
smohammadi1958@yahoo.co.uk

QR Code for Mobile users

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Using Klein Gordon Equation to Study Spin Zero Atoms

Saeed Mohammadi, Maryam Mounesi
Department of Physics, Payame Noor University, PO BOX 19395-3697 Tehran, Iran.

ABSTRACT

Klein Gordon equation is a useful dynamical equation for a certain class of particles. A problem arises however in the probabilistic interpretation of its solutions as representing a single particle. The difficulty with the Klein Gordon equation is that it has both positive and negative energy solutions. This can be shown to give rise to antiparticles which must be included for self consistency.
The Klein Gordon equation can be used to solve the hydrogen atom problem in a relativistically correct way; it is only appropriate for spin-0 particles, and thus does not apply directly to electrons and the real hydrogen atom. It is useful for pionic (π) and kaonic (K) atoms, and does give some idea of the form of the relativistic corrections.

Keywords: Klein-Gordon equation, Spin-0 particles, Pionic atoms, Photons.

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INTRODUCTION

A pionic atom is an ordinary atom with one of the electrons replaced by a negative pion. These systems have been studied for fifty years but only recently has an investigation of the deeply bound states been initiated. Prior to the mid-eighties it was believed that, due to the nuclear absorption, the deeply bound pionic states were too broad to be distinguishable. However, subsequent calculations predicted that the repulsive part of the pion-nucleus optical potential pushes the pion outward, leading to a smaller overlap between the nucleus and pionic wave-function [Friedman 1985, Toki 1988, Umemoto 2000, Yamazaki 1998]. Hence, the absorption probability is decreased and even the deepest bound states are long-lived enough to be distinguishable, having widths smaller than the separation between adjacent levels.

Pionic atoms have been studied by stopping π^- beams in a target and observing the photons emitted from pionic transitions to lower levels. However, with this method it is not possible to study the deepest bound pionic states of heavy atoms since the probability is too large for the pion being absorbed by the nucleus before reaching these states. In order to study the lowest levels, the pion must be produced directly in a deeply bound state, and various reactions have been proposed and attempted for this purpose.

The first, and so far only, observation of deeply bound pionic states was accomplished in an experiment using the reaction $^{208}Pb(d, {}^{3}He){}^{207}Pb \otimes \pi^-$. In order to achieve a high energy resolution, a thin target, 50 mg/cm^2 of enriched ^{208}Pb, was used. [Gilg 2000, Itahashi 2000].

A calculation of the $^{208}Pb\ (\gamma, P)\ {}^{207}Pb \otimes \pi^-$ reaction leading to deeply bound pionic states has recently been performed. The calculation was performed for a photon energy of 170 MeV [Hirenzaki 2002].

In this article, we used Klein-Gordon equation to obtain the energy states of a free particle of spin 0. The relativistic relationship between the energy E and momentum **p** of a free particle of rest mass m is

$$E^2 = m^2c^4 + \mathbf{p}^2c^2 \qquad (1)$$

Making the substitutions

$$E \rightarrow E_{op} = i\hbar\, \partial/\partial t, \qquad \mathbf{p} \rightarrow \mathbf{p}_{op} = -i\hbar \nabla \qquad (2)$$

And acting on both sides of equation (1) on a wave function Ψ, we obtain the Schrödinger relativistic equation or Klein-Gordon equation for a free particle:

$$-\hbar^2\partial^2 \Psi /\partial t^2 = m^2c^4\, \Psi - \hbar^2c^2 \nabla^2\, \Psi \qquad (3)$$

It is worth noting that this is a second order differential equation with respect to time, in contrast to the non relativistic Schrödinger equation, which is of first order in the time derivative $\partial/\partial t$. To follow the time evolution, the Klein Gordon equation requires that both the wave function and its time derivative be specified initially, and it is not obvious how one reconciles such an evolution with that implied by a first order equation for which only the wave function itself needs to be specified initially. Another difficulty with the Klein Gordon equation is that it has both positive and negative energy solutions. The currently accepted interpretation is that the negative energy solutions describe antiparticles, and that the two initial conditions that need to be imposed are equivalent to specifying the initial values of the wave functions for the particles and the antiparticles [Greiner 1990].

Historically this was one of the difficulties in the interpretation of the Klein Gordon equation. Dirac suggested that the negative energy solutions could be interpreted physically by postulating that in the vacuum all negative energy states are filled. This is sometimes called the sea of negative energy states. Dirac suggested that a sufficiently energetic photon ($E = \hbar\omega > 2mc^2$) could knock an electron from the negative energy sea into a positive energy state. This produces an electron and a hole. The hole acts like a positively charged electron. Dirac's hole theory thus predicts the existence of the positron, which is an anti-electron. It is now accepted that every particle has a corresponding antiparticle, with the only exceptions being strictly neutral particles, which are their own antiparticle [Greiner 1990].

2. Charged particle in an electromagnetic field

If the spinless particle has an electric charge q, and moving in an electromagnetic field described by a vector potential **A**(**r**, t) and a scalar potential Φ(**r**, t), we can in analogy with the non-relativistic case make the replacements [Gasiorowicz 2003],

$$E \rightarrow E - q\Phi, \qquad \mathbf{p} \rightarrow \mathbf{p} - q\mathbf{A}$$

So that equation (1) is replaced by

$$(E - q\Phi)^2 = m^2c^4 + c^2\,(\mathbf{p} - q\mathbf{A})^2 \qquad (4)$$

Again, making the substitutions (2) and operating on both sides of (4) on a wave function Ψ (**r**, t), we obtain the Klein-Gordon equation for a spinless particle of charge q in an electromagnetic field:

$$(i\hbar\, \partial/\partial t - q\Phi)^2\, \Psi(\mathbf{r}, t) = m^2c^4\, \Psi(\mathbf{r}, t) + c^2\, (-i\hbar\, \nabla - q\mathbf{A})^2\, \Psi(\mathbf{r}, t) \qquad (5)$$

3. Stationary state solutions

Suppose that **A** and Φ are independent of the time. We may then look for stationary state solutions of equation (5), which have the form.

$$\Psi(\mathbf{r}, t) = \Psi(\mathbf{r}) \exp(-iEt/\hbar) \qquad (6)$$

Substituting (6) into (5), we obtain

$$c^2\, (-i\hbar\, \nabla - q\mathbf{A})^2\, \Psi(\mathbf{r}) = [(E - q\Phi)^2 - m^2c^4]\, \Psi(\mathbf{r}) \qquad (7)$$

In particular, if **A** = 0 and Φ is spherical symmetric, we have

$$-c^2\hbar^2 \nabla^2\, \Psi(\mathbf{r}) = [(E - q\,\Phi))^2 - m^2c^4]\, \Psi(\mathbf{r}) \qquad (8)$$

We can separate this equation in spherical polar coordinates. We write

$$\Psi_{E\ell m}(\mathbf{r}) = R_{E\ell}(r)\, Y_{\ell m}(\theta, \phi) \qquad (9)$$

and obtain for the radial functions $R_{E\ell}(r)$, the equation

$$-c^2\hbar^2\, [(d^2/dr^2 + (2/r)\, d/dr) - \ell\,(\ell+1)/r^2]\, R_{E\ell}(r) = [(E - q\Phi)^2 - m^2c^4]\, R_{E\ell}(r) \qquad (10)$$

4. Energy Levels

Using the Klein-Gordon equation (10), we want to find to find the energy levels for a spinless particle of mass m and charge q moving in the Coulomb field of a heavy nucleus of charge Zq [$\Phi(r) = -Zq^2/(4\pi\varepsilon_o r)$]. By defining the quantities

$$\beta = 2\,(E^2 - m^2c^4)^{1/2} / (\hbar c)$$

$$\lambda = (2Z\alpha mc^2)/ (\hbar c\beta) \qquad (11)$$

$$\rho = \beta r$$

$$\ell'\,(\ell'+1) = \ell\,(\ell+1) - Z^2\alpha^2$$

where $\alpha = e^2/ (4\pi\varepsilon_o\hbar c)$ is the fine structure constant, we can show that the radial Klein-Gordon equation (10) can be written in the following form,

$$[d^2/d\rho^2 - \ell'\,(\ell'+1) / \rho^2 + \lambda/\rho - ¼]\, U_{E\ell}(\rho) = 0 \qquad (12)$$

Where $U_{E\ell}(\rho) = \rho\, R_{E\ell}(\rho)$

Now equation (12) is in a form which is similar to differential equation for hydrogen atom in non-relativistic case and the method of solving it is by Laguerre polynomials which can be found in any textbooks on quantum mechanics, for example look at references [Gasiorowicz 2003 and Robinett 2006]. It can be shown that the condition for the power series solution to terminate is

$$\lambda = n + \ell' + 1 \qquad (13)$$

Putting instead of λ and ℓ' from equations (11), we can show that the quantized energies now depend on both **n** and **ℓ** (in contrast to the non-relativistic case), and are given by

$$E_{n,\ell} = mc^2\, \{1 + (Z\alpha)^2/ [n + ((\ell + ½)^2 - (Z\alpha)^2)^{½} - (\ell + ½)]^2\}^{-½} \qquad (14)$$

if we expand the above result in power of $(Z\alpha)$, we can show that

$$E_{n,\ell} = mc^2\, \{1 - (Z\alpha)^2\, [1 + (Z\alpha)^2\, (1/ (\ell + ½) - 3/4n) / n + \ldots]/2n^2\} \qquad (15)$$

or

$$E_{n,\ell} = mc^2 - ½\, mc^2\, (Z\alpha)^2/n^2 - \ldots \qquad (16)$$

That is, to first order in $(Z\alpha)$, the energies are quantized in terms of n, and the second order term which is proportional to $(Z\alpha)^4$, is related to relativistic corrections to energies.

Now we consider the applications of the Klein-Gordon equation for some 0 spin particles.

4.1. π mesons

Charged pions $\pi^{\pm}$ have masses of 140 MeV/c^2, and a neutral pion π^o was later discovered that has a mass of 135 MeV/c^2 [4]. Thus, the rest mass of π mesons is $m_\pi \approx 260\, m_e$, so that to first order in $(Z\alpha)$, the energies of a pionic atom are,

$$E_n = -260 \times 13.6Z^2/n^2$$

4.2. Photons

Since photons have m = 0 and q = 0, equation (8) reduces to,

$$\nabla^2\, \Psi(\mathbf{r}) - (1/c^2)\, \partial^2\Psi /\partial t^2 = 0$$

Which is appropriate to the propagation of electromagnetic fields in vacuum, for either the scalar or vector potential [Jackson 1999].

CONCLUSIONS

We used Klein Gordon equation to solve for pionic atoms, which are particles with 0 spin, and showed that the negative energy solutions could be interpreted physically as antiparticles. Another success of this equation is that it can be used for photons which have 0 spin and rest mass. In this case it reduces to the propagation of electromagnetic fields in vacuum.

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