Perturbations for the Coulomb - Kepler problem on de Sitter space-time

Pop Adrian Alin

West University of Timişoara, V. Pârvan Ave. 4, RO-300223 Timişoara, Romania

Abstract

In the Schrödinger picture of the Dirac quantum mechanics, defined in charts with spatially flat Robertson-Walker metrics and Cartesian coordinates the perturbation theory is applied to the interacting part of the Hamiltonian operator produced by the minimal coupling with the gravitational field. First and second order perturbations are computed.

Key words: perturbations; de Sitter space-time; Schrödinger picture; gravitational field; hydrogen atom;

1 Introduction

The purpose of this paper is to investigate the possible influences of the gravitational field over a system such as the hydrogen atom in a de Sitter spacetime. Do such influences exist and if so, are these measurable by any experiment ?

Recently a new time-evolution picture of the Dirac quantum mechanics was defined in charts with spatially flat Robertson-Walker metrics, under the name of Schrödinger picture [1]. In the non-relativistic quantum mechanics the time evolution can be studied in different pictures (e. g., Schrödinger, Heisenberg, Interaction) which transform among themselves through specific time-dependent unitary transformations. It is known that the form of the Hamiltonian operator and the time dependence of other operators strongly depend on the picture choice. In special and general relativity, despite of its importance, the problem of time-evolution pictures is less studied because of

Email address: apop302@quantum.physics.uvt.ro (Pop Adrian Alin).

the difficulties in finding suitable Hamiltonian operators for scalar or vector fields.

We are interested in the Schrödinger picture defined in charts with spatially flat Robertson-Walker metrics and Cartesian coordinates. We take a look at the Schrödinger equation in this picture. On a space-time with Robertson-Walker metric the Coulomb potential has the form $\frac{q^2}{r}\alpha(t)$. In the moving charts with RW metrics of the de Sitter spacetime the operator H(t) is timeindependent and $\dot{\alpha}/\alpha = \text{const.}$ In this conditions the Coulomb potential in the Schrödinger picture is just $\frac{q^2}{r}$ so we find that the Schrödinger equation for the hydrogen atom is identical with the one from the non-relativistic quantum mechanics. This is the perfect scenario to apply the perturbation theory.

Trying to add the gravitational interaction to the simple problem of the hydrogen atom gives us a very interesting case to study. The Coulomb - Kepler problem is not solved directly so far by the use of the Dirac or Schrödinger equations. We propose to study the effects of the gravitational interaction by considering gravity as a perturbation added to the simpler problem of the hydrogen atom. For this paper we use numerical methods to compute the perturbations for the energy levels produced by the minimal coupling with the gravitational field. We set the entire problem on the de Sitter space-time and apply the perturbation theory.

We start in the second section with a presentation of the Schrödinger picture and by writing down the Schrödinger equation we will be using and an explanation of why it has this form in our particular case. The next section is devoted to the perturbation theory and how we applied it in our case. A brief description of the numerical method used is also given as well as the results that were obtained with it. In the last section we are drawing a conclusion from these results.

2 Preliminaries

We consider the Schrödinger picture as the picture in which the kinetic part of the Dirac operator takes the standard form $i\gamma^0\partial_t + i\gamma^i\partial_i$ [1]. The transformation $\psi(x) \rightarrow \psi_S(x) = U_S(x)\psi(x)$ leading to the Schrödinger picture is produced by the operator of time dependent *dilatations*

$$U_S(x) = \exp\left[-\ln(\alpha(t))(\vec{x} \cdot \vec{\partial})\right], \qquad (1)$$

The Schrödinger picture may offer one some technical advantages in solving problems of quantum systems interacting with the gravitational field. For example, in this picture we can derive the non-relativistic limit (in the sense of special relativity) replacing \mathcal{H}_0 directly by the Schrödinger kinetic term $\frac{1}{2m}\vec{P}_S^2$, where the Hamiltonian operator $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int}$. Thus we obtain the Schrödinger equation

$$\left[-\frac{1}{2m}\Delta - i\frac{\dot{\alpha}(t)}{\alpha(t)}\left(\vec{x}\cdot\vec{\partial} + \frac{3}{2}\right)\right]\phi(x) = i\partial_t\phi(x)\,,\tag{2}$$

for the wave-function ϕ of a spinless particle of mass m.

In the particular case of the de Sitter spacetime, the Schrödinger picture will lead to important new results for the Schrödinger equation in moving charts with RW metrics and spherical coordinates. In these charts where H = H(t)is conserved, the mentioned equation (2) is analytically solvable in terms of Whittaker hypergeometric functions.

We consider the interaction hamiltonian term $\mathcal{H}_{int} = \vec{x} \cdot \vec{\partial} + \frac{3}{2}$ as a perturbation and would like to apply the well known methods of the perturbation theory to a simple case like the hydrogen atom. Our equation in physical units is

$$\left[-\frac{\hbar^2}{2m}\Delta - i\hbar\omega\left(\vec{x}\cdot\vec{\partial} + \frac{3}{2}\right) + \frac{q^2}{r}\right]\Psi(x) = E\Psi(x)\,,\tag{3}$$

where $q^2 = \frac{Ze^2}{4\pi\epsilon_0}$ is the Coulomb potential (and Z = 1 for the hydrogen atom). It can be easily shown that on de Sitter space-time the Coulomb potential has the same form $\left(\frac{q^2}{r}\right)$ as on Minkowski space-time; in this way the "clasical" problem of the hydrogen atom remains unchanged and the perturbation theory is well suited for studying the effects of minimal coupling with the gravitational field.

3 Perturbations - first and second order

It is obviously much better for such a case as the hydrogen atom to work with spherical coordinates. Making the transformation $\{t, \vec{x}\} \rightarrow \{t, r, \theta, \phi\}$ we get $\vec{r}\vec{\partial} = r\frac{\partial}{\partial r}$. We also have the possibility now to separate the radial components from the spherical components:

$$\langle \vec{x}|n,l,m\rangle = \langle r,\theta,\phi|n,l,m\rangle; \Psi(r,\theta,\phi) = R_{nl}(r)Y_{lm}(\theta,\phi)$$
(4)

The radial functions are well known and can be expressed in terms of the Laguerre polynoms:

$$R_{nl}(r) = -\left\{\frac{2Z}{na_0}\frac{(n-l-1)!}{2n[(n+l)!]^3}\right\}^{\frac{1}{2}}e^{(-\frac{\rho}{2})}\rho^l L_{n+l}^{2l+1}(\rho)$$
(5)

where $\rho = \frac{2Z}{na}r$. The angular components of $\Psi(r, \theta, \phi)$ have to satisfy the condition $\int Y_{lm}^* Y_{l'm'} d\Omega = \delta_{ll'} \delta_{mm'}$ so we will only have to deal with the radial components from this point on.

The energy levels in the case of the hydrogen atom are given by $E_n^{(0)} = \frac{me_0^4}{2\hbar^2} \frac{1}{n^2}$; by adding corrections due to perturbations we have

$$\Delta E = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots$$

. We want to compute this corrections for the first and second order. For the first order we just need the matrix elements of the interacting hamiltonian term.

$$E_n^{(1)} = < n, l, m | H_{int} | n'l'm' >$$
(6)

The computation is straightforward and the result is zero for any value of n (energy level). This means the first order perturbations give no contribution to the correction of the energy levels.

For the second order we used the well known relations from the perturbation theory that give us the second order perturbations of the energy levels.

$$E_n^{(2)} = \sum_{k \neq n} \frac{\langle E_n | H_{int} | E_k \rangle \langle E_k | H_{int} | E_n \rangle}{E_n - E_k}$$
(7)

This time te computation gets more complicated but still solvable with a mathematical software like Maple or Mathematica or by implementing a custom numerical routine. We define a procedure that can compute the values of the radial functions using the Laguerre polynoms by taking as input only the values of the quantum numbers n and l. Using this we write the action of H_{int} over $|E_k\rangle$ and we can evaluate the integrals from the equation (7). Than is just a matter of making the summation of the terms of this equation omitting the term where $k \neq n$. By controling the number of terms in this summation we cand adjust the precision of our method. The contributions due to the second order perturbations are not zero like those of the first order.

We will give hear the results for the first values of n that were obtained with some custom Maple procedures, with Z = 1 for the hydrogen atom. We have

$$E_n^{(2)} = \frac{\hbar^4 \omega^2}{m e_0^4} \epsilon^{(2)} \tag{8}$$

to get to a system of units with physical meaning. Bellow are given some of the computed values for the dimensionless quantity $\epsilon^{(2)}$.

n	1	Number of terms				
		10	30	50	100	1000
1	0	1.064095523	1.073619436	1.074421747	1.074765599	1.074880495
2	0	18.46605472	18.67877161	18.69583748	18.70311224	18.70553792
2	1	13.70700332	13.83414505	13.84427053	13.84858330	13.85002081
3	0	95.93893645	97.31876631	97.42041641	97.46335870	97.47762648
3	1	84.69291072	85.74907706	85.82617976	85.85872010	85.86952714
3	2	60.91483176	61.40294550	61.43776962	61.45243081	61.45729539
4	0	305.9528653	311.5523974	311.9151219	312.0664192	312.1164354
4	1	285.5680992	290.2868876	290.5892387	290.7152100	290.7568349
4	2	243.4746022	246.5590712	246.7515894	246.8315844	246.8579881
4	3	177.1352766	178.3299632	178.4009022	178.4302308	178.4398912
4 4 Table	2 3	243.4746022 177.1352766	246.5590712 178.3299632	246.7515894 178.4009022	246.8315844 178.4302308	246.857988 178.43989

Perturbation for the energy levels $\epsilon_n^{(2)}$ computed with different number of terms

For the equation (7) the same numerical routines were applied making the sumation for different number of terms, from 10 to 1000. This was a test of the convergence of our method of computation; the results did not change significantly even though the number of terms was greatly increased.

We ask ourselves what is the magnitude of this perturbation in order to see if it can be measured or not, and if so what to expect. For this we evaluate from the equation (8) the factor that multiplies $\epsilon^{(2)}$ by having the value of ω of the same order as the Hubble constant $(H_0 \approx 2.3 \times 10^{-18} s^{-1})$ in our de Sitter universe. This gives us : $\frac{\hbar^4 \omega^2}{m e_0^4} = \frac{(\hbar \omega)^2}{1u.a.e} \approx 8.4 \times 10^{-68} eV$ (1u.a.e. = 27.21 eV). This value is extremely small and obviously can not be measured in any experiment.

4 Concluding remarks

Let us summarize what was done: we have started with the classical hydrogen atom problem by taking advantage of the fact that on de Sitter space-time the Coulomb potential has the same form as on Minkowski space-time. We have considered the gravitational interaction as a perturbation and using the perturbation theory we have computed the first and second order perturbations for the energy levels of the atom. In the first order we have seen that all this are zero. In the second order although we got non-zero values those are so small that can easily be neglected and can not be even measured in any kind of experiment. The conclusion we draw is that theere are no measurable cosmological influences over the atoms from the minimal coupling with the gravitational field.

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