Quantum Dynamics of Atomic Electrons

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Abstract

In this Thesis we study the Quantum Dynamics of Atomic Electrons. Using the mathematical derivation of the system of two coupled differential equations for the radial wave function, we have calculated the Sommerfeld expression for energy eigenvalues for electrons bound to nuclei. Then we have calculated the wave function at the diving point. Applying the Sommerfeld-fine structure formula, we have calculated the binding energies for $1s_{1/2}$. And we have classified the bound states of the electron according to the Dirac equation for $Z = 1$ (hydrogen atom). We found that the energy levels descend progressively with increasing Z. The energy of the lowest state $(1s, k = 1)$ becomes negative when the nuclear charge $Z > 150$ and $1s$ level finally reaches the values $E_{1s} = -m_0c^2$ at a critical charge $Z_{cr}^{1s} \simeq 173$. Hence the Sommerfeld energies of the states with $k = -1(ns_{1/2})$ and $k = +1(np_{1/2})$ break off with a vertical tangent at $Z\alpha = 1$ and with the finite nuclear radius taken into account all levels reach the edge of the lower continuum $E = -m_0c^2$ at a corresponding critical charge Z_{cr}.

Using perturbation potential V' we have determined the Fano's formalism for the description of resonances. And using Fano's formalism we have calculated the final hole probability in the bound state and the spectrum of the emitted positrons depending on the diving duration. Then, we found that the modified continuum wave $\Psi_E(r)$ thus displays exactly the same asymptotic behavior as $\psi_E(r)$ but it is shifted by an angle Δ_E. The probability of finding a hole in state ϕ_0 after a time T thus decreases exponentially as determined by the decay width $\Gamma_0 = \Gamma_{E_r}$. An oscillating function with maximum at $E = E_r$ having a width decreasing with the inverse of T. The peak height increases quadratically and it consistent linearly in T until saturation is reached at $T > 1/\Gamma_0$.

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Chapter 1

Introduction

Quantum electrodynamics (QED) is the theory that describes the interactions of photons with electrons [1]. It is the most precise theory in all of science, which means that it makes quantitative predictions that have been verified experimentally to remarkable accuracy [4-6]. QED is also the starting point for all theoretical treatment of elementary particles. The strong and weak interactions are modeled after the interactions of electrons and photons [2,13,14,16]. QED is one of the most well tested, accurate, and successful theories in physics [7,15].

QED is so accurate and all-encompassing that it can't be at all wrong, but it does leave us with a number of puzzles and paradoxes.

- Truly elementary particles have mass, spin, and other additive quantum numbers like charge, baryon number, lepton number, etc., but they have no size; they are point-like objects. How, for example, can something with no size have spin?

- Some interaction terms that appear inevitably when doing perturbation theory lead to divergent integrals. Taming of these integrals is by the methed of renormalization.

So on one hand, QED is a sturdy computational tool that should be part of the knowledge base of any real physicist. On the other, it is a doorway to many of the unsolved problems of modern physics [8,9].

According to QED, charged particles interact with one other by emitting or absorbing photons, which are the carriers of the electromagnetic force. QED correctly predicts such phenomena as the structure of atoms, and the creation and annihilation of particles (for example, when matter and antimatter collide) [10,11,12].

In this thesis we try to provide a good working knowledge of QED of strong fields generally and Quantum Dynamics of Atomic Electrons particularly. To this end, we first introduce the mathematical derivations of the system of two coupled differential equations for the radial wave function from the Hamiltonian of the Dirac equation with central potential. Then we develop Sommerfeld expression for energy eigenvalues for electrons bound to nuclei from the coupled radial equations. From this we are able to derive the wave function at the Diving point, and then we discuss the Sommerfeld fine-structure formula and the classification of the electron levels. Finally, we deal with the Fanos formalism for the description of resonances and time-dependent decay of the vacuum.

Chapter 2

Derivation of System of Two Coupled Differential Equations

Nature provides atomic nuclei as an almost ideal source of strong external electric field. A nucleus of charge Z and a mass number A produces a spherically symmetric potential of the form

$$V(r) = ZU(r) = \begin{cases} -Ze^2/r, & for\ r > R \\ -(Ze^2/R)f(r), & for\ r < R. \end{cases} \tag{2.0.1}$$

If the nucleus is consider as a homogeneously charged sphere with a sharp edge, which is sufficient for most purposes, then the bottom of the potential well is parabolic, i.e.

$$f(r) = \frac{1}{2}(3 - \frac{r^2}{R^2}),$$

but simple approximation we uses $f(r) = 1$, corresponding to a charged spherical shell. The Hamiltonian for the Dirac equation with central potential is given by

$$\hat{H}_D = c\hat{\alpha}.\,\hat{p} + \hat{\beta}m_0c^2 + V(r), \tag{2.0.2}$$

where $V(r) = eA_0(r)$. Because of the spherical symmetry of the field, the angular momentum operator $\hat{J}$ and the parity operator $\hat{P} = e^{i\varphi}\hat{\beta}(x \longrightarrow -x) = e^{i\varphi}\gamma^0\hat{P}_0$ with respect to the origin of the coordinate system commute with the Hamiltonian. Hence states with definite energy, angular momentum and parity occur. The corresponding wave functions

are denoted by

$$\psi_{jm} \quad = \begin{pmatrix} \varphi_{jlm}(x,t) \\ \chi_{jl'm}(x,t) \end{pmatrix}. \tag{2.0.3}$$

Here φ_{jlm} and $\chi_{jl'}$ are two-spinor which are to be determined. Since ψ_{jm} must have good parity and the parity operator is given by $\hat{P} = e^{i\varphi}\hat{\beta}\hat{P}_0$ ($\hat{P}_0$ changes x to -x) and we obtain

$$\psi'_{jm}(x',t') = \lambda\psi_{jm}(x',t') \quad or \quad \hat{P}\psi_{jm}(x') = \lambda\psi_{jm}(x',t'), \tag{2.0.4}$$

$$\begin{aligned} \hat{P}\psi_{jm} \quad &= e^{i\varphi}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\ \hat{P}_0\begin{pmatrix} \varphi_{jlm}(x,t) \\ \chi_{jl'm}(x,t) \end{pmatrix} = e^{i\varphi}\begin{pmatrix} \hat{P}_0\varphi_{jlm}(x,t) \\ -\hat{P}_0\chi_{jl'm}(x,t) \end{pmatrix} \\ &= \lambda\psi_{jm} = \lambda\begin{pmatrix} \varphi_{jlm}(x,t) \\ \chi_{jl'm}(x,t) \end{pmatrix}. \end{aligned} \tag{2.0.5}$$

Eq. (2.0.5) shows that the parity of the two spinor φ_{jlm} must be equal to the negative parity of $\chi_{jl'm}$. We can also understand this statement in the following way; which is the stationary Dirac equation $\hat{H}_D\psi = E\varphi$, we get with

$$\hat{\alpha} = \begin{pmatrix} 0 & \hat{\sigma} \\ \hat{\sigma} & 0 \end{pmatrix}$$

that

$$\begin{aligned} c(\hat{\sigma}\cdot\hat{p})\chi + m_0c^2\varphi + V\varphi = E\varphi, \\ c(\hat{\sigma}\cdot\hat{p})\varphi - m_0c^2\chi + V\chi = E\chi. \end{aligned} \tag{2.0.6}$$

or

$$\begin{aligned} (E - m_0c^2 - V)\varphi = c(\hat{\sigma}\cdot\hat{p})\chi, \\ (E + m_0c^2 - V)\chi = c(\hat{\sigma}\cdot\hat{p})\varphi. \end{aligned} \tag{2.0.7}$$

Since the operate $\hat{\sigma}\cdot\hat{p}$ changes parity, these equations show that the two spinors φ and χ must have opposite parity.

Eigenfunctions of the angular momentum and the parity operator are the well known spherical spinors. To avoid confusion with the complete wave function Ψ we shall denote the spherical spinors here by Ω_{jlm}. They are defined by

$$\Omega_{jlm} = \sum_{m'm_s} (l\frac{1}{2}j|m'm_sm)Y_{lm'}\chi_{\frac{1}{2}m_s}. \tag{2.0.8}$$

Here the two spinor $\chi_{\frac{1}{2}m_s}$ are eigenfunctions of the spin operators $\hat{S}^2 = \hat{\hbar}^2\hat{\sigma}^2/4$ and $\hat{S}_3 = \hbar\hat{\sigma}_3/2$; they are given explicitly as
$\chi_{\frac{1}{2}\frac{1}{2}} = \begin{pmatrix}1\\0\end{pmatrix}$, $\chi_{\frac{1}{2}\frac{-1}{2}} = \begin{pmatrix}0\\1\end{pmatrix}$
The parity of Ω_{jlm} is given by Y_{lm}:

$$\hat{P}_0\Omega_{jlm} = (-1)^l\Omega_{jlm}. \tag{2.0.9}$$

We make the following ansatz

$$\begin{aligned}\varphi_{jlm} &= ig(r)\Omega_{jlm}(\mathbf{r}/r),\\ \chi_{jl'm} &= -f(r)\Omega_{jl'm}(\mathbf{r}/r).\end{aligned} \tag{2.0.10}$$

with

$$l' = 2j - l = \begin{cases}2(l+\frac{1}{2}) - l = l+1, & for\ j = l+\frac{1}{2},\\ 2(l-\frac{1}{2}) - l = l-1, & for\ j = l-\frac{1}{2}.\end{cases} \tag{2.0.11}$$

If $j = l+1/2$, the orbital angular momentum l' of $\chi_{jl'm}$ is $l' = l+1$. This is the only way to realize the opposite parity of χ compared to φ. The Value $l' = l-1$ must be excluded, because no total angular momentum $j = l+\frac{1}{2}$ can be constructed by $l' = l-1$ and $S = \frac{1}{2}$. The arguments follow a similar pattern for the second case of Eq. (2.0.11)
and we have

$$\begin{aligned}\hat{\sigma}\cdot\hat{p}\varphi_{jlm} &= \hat{\sigma}\cdot\hat{p}\Big(ig(r)\Omega_{jlm}(\mathbf{r}/r)\Big)\\ &= (\hat{\sigma}\cdot\hat{p}ig(r))\Omega_{jlm} + ig(r)\hat{\sigma}\cdot\hat{p}\Omega_{jlm}\\ &= \hbar\frac{dg(r)}{dr}\Big(\hat{\sigma}\cdot\mathbf{r}/r\Big)\Omega_{jlm} + ig(r)\hat{\sigma}\cdot p\Omega_{jlm}.\end{aligned} \tag{2.0.12}$$

With respect to Eq. (2.0.8) the spherical spinors are eigenfunctions of the operators $\hat{L^2}$, $\hat{J^2}$ and $\hat{S^2} = (\frac{1}{2}\hat{\sigma})^2$ with eigenvalues $l'(l'+1)\hbar^2$, $j(j+1)\hbar^2$ and $\frac{3}{4}\hbar^2$ respectively. In order to be complete we once more give the explicit form of the Ω_{jlm} for the useful cases $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$ $(j \geq \frac{1}{2})$

$$\Omega_{\underbrace{l+\frac{1}{2}}_{j},l,m} = \begin{pmatrix} \sqrt{\frac{j+m}{2j}} Y_{l,m-\frac{1}{2}} \\ \sqrt{\frac{j-m}{2j}} Y_{l,m+\frac{1}{2}} \end{pmatrix}, \tag{2.0.13}$$

$$\Omega_{\underbrace{l-\frac{1}{2}}_{j},l,m} = \begin{pmatrix} -\sqrt{\frac{j-m+1}{2j+2}} Y_{l,m-\frac{1}{2}} \\ \sqrt{\frac{j+m+1}{2j+2}} Y_{l,m+\frac{1}{2}} \end{pmatrix}. \tag{2.0.14}$$

The root factors Eqs. (2.0.13) and (2.0.14) are the Glebsch-Gordon coefficients in explicit form. Now we make use of the following relation between the spherical spinors

$$(\hat{\sigma}\cdot\frac{\mathbf{r}}{r})\Omega_{jl'm} = -\Omega_{jl'm}, \tag{2.0.15}$$

$(\hat{\sigma}\cdot\frac{\mathbf{r}}{r})$ is a scalar operator of negative parity and if multiply with Eq. (2.0.15) we get

$$-(\hat{\sigma}\cdot\hat{p})\Omega_{jlm} = (\hat{\sigma}\cdot\hat{p})(\hat{\sigma}\cdot\frac{\mathbf{r}}{r})\Omega_{jl'm}. \tag{2.0.16}$$

and we have the relation

$$(\hat{\sigma}\cdot\mathbf{A})(\hat{\sigma}\cdot\mathbf{B}) = \mathbf{A}\cdot\mathbf{B} + i\hat{\sigma}\cdot(\mathbf{A}\times\mathbf{B}), \tag{2.0.17}$$

to change Eq. (2.0.16) into

$$-(\hat{\sigma}\cdot\hat{p})\Omega_{jlm} = \left(\hat{p}\cdot\frac{\mathbf{r}}{r} + i\hat{\sigma}\cdot(\hat{p}\times\frac{\mathbf{r}}{r})\right)\Omega_{jl'm}. \tag{2.0.18}$$

With $\hat{p} = i\hbar\nabla$ and $\hat{L} = r\times\hat{p}$, Eq. (2.0.18) can further be transformed into

$$\begin{aligned}
&(\hat{p}\cdot\mathbf{r} + i\hat{\sigma}\cdot(\hat{p}\times\mathbf{r}))\frac{1}{r}\Omega_{jl'm} \\
&= \left(-i\hbar(\nabla\cdot\mathbf{r}) - i\hbar\mathbf{r}\cdot\nabla - i\hat{\sigma}\cdot(\mathbf{r}\times\hat{p})\right)\frac{1}{r}\Omega_{jl'm} \\
&= \left(-i\hbar\frac{3}{r} - i\hbar\mathbf{r}(-\frac{1}{r^2}) - i\frac{\hat{\sigma}\cdot\hat{L}}{r}\right)\Omega_{jl'm} \\
&= -i\left(\frac{2\hbar}{r} + \frac{1}{r}\hat{L}\cdot\hat{\sigma}\right)\Omega_{jl'm}.
\end{aligned} \tag{2.0.19}$$

And we have

$$\hat{J}^2 = (\hat{L} + \frac{\hbar}{2}\hat{\sigma})^2 = \hat{L}^2 + (\frac{\hbar}{2}\hat{\sigma})^2 + \hbar\hat{\sigma}\cdot\hat{L}. \tag{2.0.20}$$

Thus, we can write,

$$\begin{aligned} \hbar\hat{L}\cdot\hat{\sigma}\,\Omega_{jl'm} &= \left(\hat{J}^2 - \hat{L}^2 - (\frac{\hbar}{2}\hat{\sigma})^2\right)\Omega_{jl'm} \\ &= \left(j(j+1) - l'(l'+1) - \frac{3}{4}\right)\hbar\Omega_{jl'm}. \end{aligned} \tag{2.0.21}$$

Now let us define a quantum number k in convenient way by

$$k = \mp(j + \frac{1}{2}) = \begin{cases} -(l+1), & for\ j = l + 1/2, \\ l, & for\ j = l - 1/2. \end{cases} \tag{2.0.22}$$

Obviously there is

$$|k| = j + 1/2 \quad or \quad j = |k| - 1/2. \tag{2.0.23}$$

With this and taking $l' = 2j - l$ into account we can rewrite the expectation value on the right hand side of Eq. (2.0.21). For $j = l + \frac{1}{2}$, we get

$$\begin{aligned} &(l + \frac{1}{2})(l + \frac{1}{2} + 1) - [2(l + \frac{1}{2}) - l][2(l + \frac{1}{2}) - l + 1] - \frac{3}{4} \\ &= l^2 + \frac{1}{2}l + l + \frac{1}{2}l + \frac{1}{4} + \frac{1}{2} - (l+1)(l+2) - \frac{3}{4} \\ &= l^2 + 2l - l^2 - 2l - l - 2 \\ &= -(l+2) \\ &= k - 1. \end{aligned} \tag{2.0.24}$$

Similarly for $j = l - \frac{1}{2}$:

$$\begin{aligned}
&(l-\frac{1}{2})(l+\frac{1}{2}) - [2(l-\frac{1}{2}) - l][2(l-\frac{1}{2}) - l + 1] - \frac{3}{4} \\
&= l^2 + \frac{1}{2}l + l - \frac{1}{2}l - \frac{1}{4} - [2l - (l+1)(2l-1-l+1) - \frac{3}{4} \\
&= l^2 - \frac{1}{4} - (l-1)l - \frac{3}{4} \\
&= l^2 - \frac{1}{4} - (l^2 - l) - \frac{3}{4} \\
&= l - \frac{1}{4} - \frac{3}{4} \\
&= l - 1 \\
&= k - 1. \qquad (2.0.25)
\end{aligned}$$

Now Eq. (2.0.19) can be written as

$$(2\hbar + \hat{L}\cdot\hat{\sigma})\Omega_{jl'm} = (1+k)\hbar\Omega_{jl'm}. \qquad (2.0.26)$$

If in Eq. (2.0.21) we had started with Ω_{jlm} we would have obtained
$(2\hbar + \hat{L}\cdot\hat{\sigma})\Omega_{jlm} = (1-k)\hbar\Omega_{jlm}$ by the same procedure. And the following notations are used for Eq. (2.0.26);

$$\chi_{k,m} \equiv \Omega_{jlm} \ \ , \ \chi_{-k,m} \equiv \Omega_{jl'm} \qquad (2.0.27)$$

we then define the operator,

$$\hat{k} = \hbar + \hat{L}\cdot\hat{\sigma}, \qquad (2.0.28)$$

so that due to Eq. (2.0.26) the eigenvalue equation

$$\hat{k}\chi_{k,m} = -\hbar k\chi_{k,m} \ \ , \ \hat{k}\chi_{-k,m} = \hbar k\chi_{-k,m} \qquad (2.0.29)$$

holds, where

$$k = \begin{cases} -(l+1) = -(j+\frac{1}{2}), & for\ j = l + \frac{1}{2}, \\ l = +(j+\frac{1}{2}), & for\ j = l - \frac{1}{2}. \end{cases} \qquad (2.0.30)$$

Consequently, the spherical spinors of Eq. (2.0.10) can also be denoted by $\chi_{k,m} = \Omega_{jlm}$ and $\chi_{-k,m} = \Omega_{jl'm}$ and we can therefore write the four-spinor in central field as

$$\begin{aligned}\psi_{jm} = & \begin{pmatrix}\varphi_{jlm}(x,t)\\ \chi_{jl'm}(x,t)\end{pmatrix} = \begin{pmatrix} ig(r)\Omega_{jlm}(\frac{\mathbf{r}}{r})\\ -f(r)\Omega_{jl'm}(\frac{\mathbf{r}}{r})\end{pmatrix}\\ = & \begin{pmatrix} ig(r)\chi_{k,m}\\ -f(r)\chi_{-k,m}\end{pmatrix} = +i\begin{pmatrix} g(r)\chi_{k,m}\\ if(r)\chi_{-k,m}\end{pmatrix}.\end{aligned}$$

With this and Eqs. (2.0.15) and (2.0.18), Eq. (2.0.12) finally takes the form

$$\hat{\sigma}\cdot\hat{p}\varphi_{jlm} = -\Omega_{jl'm}\left(\hbar\frac{dg}{dr} + \frac{k+1}{r}\hbar g(r)\right). \tag{2.0.31}$$

and

$$\hat{\sigma}\cdot\hat{p}\chi_{jl'm} = -\Omega_{jlm}\left(\hbar\frac{df(r)}{dr} - \frac{k-1}{r}\hbar f(r)\right). \tag{2.0.32}$$

Now by inserting the expressions of Eqs. (2.0.31) and (2.0.32) in Eq. (2.0.7), the angular functions from both sides of the equation can be eliminated. So we obtain the differential equations for the radial function f and g:

$$\begin{aligned}\hbar c\frac{dg(r)}{dr} + (1+k)\hbar c\frac{g(r)}{r} - [E + m_o c^2 - V(r)]f(r) = 0,\\ \hbar c\frac{df(r)}{dr} + (1-k)\hbar c\frac{f(r)}{r} + [E - m_o c^2 - V(r)]g(r) = 0.\end{aligned} \tag{2.0.33}$$

With substitution $u_1 = rg$ and $u_2 = rf$ with

$$\frac{du_1(r)}{dr} = g + r\frac{dg(r)}{dr},$$

and

$$\frac{du_2}{dr}(r) = f + r\frac{df(r)}{dr}.$$

Finally we get

$$\begin{aligned}\hbar c\frac{du_1(r)}{dr} + \hbar c\frac{k}{r}u_1(r) - [E + m_0 c^2 - V(r)]u_2(r) = 0,\\ \hbar c\frac{du_2(r)}{dr} - \hbar c\frac{k}{r}u_2(r) + [E - m_0 c^2 - V(r)]u_1(r) = 0.\end{aligned} \tag{2.0.34}$$

These are the coupled differential equations for the radial wave function u_1 and u_2 of the Dirac equation in the case of a spherically symmetric potential $V(r)$.

The system of two coupled ordinary differential equation of the first order ($\hbar = c = 1$) is reduced to

$$\begin{aligned} \frac{d}{dr}u_1(r) &= -\frac{k}{r}u_1(r) + [E + m_0 - V(r)]u_2(r), \\ \frac{d}{dr}u_2(r) &= \frac{k}{r}u_2(r) - [E - m_0 - V(r)]u_1(r). \end{aligned} \tag{2.0.35}$$

For all energies $E > m_0$, and $E < m_0$, Eq. (2.0.35) possesses continuum solutions which are regular at the origin ($r = 0$) and oscillate asymptotically ($r \to \infty$). In the energy gap $-m_0 < E < m_0$ only at certain discrete energy the eigenvalues E_{nj}, are solutions found that fulfill the regularity requirement at $r \to 0$ and $r \to \infty$ simultaneously and are thus normalizable.

Chapter 3

Derivation of Sommerfeld Expression for Energy Eigenvalues for Electrons Bound to Nuclei

We now seek to study the Sommerfeld expression for energy eigenvalues for electrons bound to nuclei, the wave function at the diving point, and the Sommerfeld fine-structure formula and the classification of the electron levels.

3.1 Coupled differential equations for a Dirac particle in a coulomb potential and the energy eigenvalues for the bound states

The coulomb interaction energy of a point nucleus and a particle of charge $-e$ is

$$V = -\frac{Ze^2}{r}.$$

So that the system of two coupled ordinary differential equation for a Dirac particle is already obtained as

$$\begin{aligned} \frac{du_1}{dr} &= -\frac{k}{r}u_1 + \left[\frac{E + m_o c^2}{\hbar c} + \frac{Ze^2}{r(\hbar c)}\right]u_2, \\ \frac{du_2}{dr} &= \frac{k}{r}u_2 - \left[\frac{E - m_o c^2}{\hbar c} + \frac{Ze^2}{r(\hbar c)}\right]u_1. \end{aligned} \tag{3.1.1}$$

But from the relation we have $\alpha = e^2/\hbar c \approx \frac{1}{137}$ is the fine-structure constant. Then Eq. (3.1.1) becomes

$$\begin{aligned} \frac{du_1}{dr} &= -\frac{k}{r}u_1 + \left[\frac{E + m_o c^2}{\hbar c} + \frac{Z\alpha}{r}\right]u_2, \\ \frac{du_2}{dr} &= \frac{k}{r}u_2 - \left[\frac{E - m_o c^2}{\hbar c} + \frac{Z\alpha}{r}\right]u_1. \end{aligned} \tag{3.1.2}$$

Now let us ex-mine the solution of the Eq. (3.1.2) for smaller r, i.e. near the origin ($r \sim 0$). In this case the term with $E \pm m_0 c^2$ can be omitted and we get

$$\begin{aligned} \frac{du_1}{dr} + \frac{k}{r}u_1 - \frac{Z\alpha}{r}u_2 = 0, \\ \frac{du_2}{dr} + \frac{k}{r}u_2 + \frac{Z\alpha}{r}\ u_1 = 0. \end{aligned} \tag{3.1.3}$$

Using a power series expansion for the solution of Eq. (3.1.3), the first term of this series dominates in the region near the origin. This motivates the ansatz $u_1 = ar^\gamma$, and $u_2 = br^\gamma$. Using this it follow that

$$\begin{aligned} a\gamma r^{\gamma-1} + \kappa a r^{\gamma-1} - Z\alpha b r^{\gamma-1} = 0, \\ b\gamma r^{\gamma-1} + \kappa b r^{\gamma-1} + Z\alpha a r^{\gamma-1} = 0. \end{aligned} \tag{3.1.4}$$

Or

$$a(\gamma + \kappa) - bZ\alpha = 0 \quad , \quad aZ\alpha + b(\gamma - \kappa) = 0. \tag{3.1.5}$$

The determinant of the coefficient must vanish, and yields

$$\gamma^2 = k^2 - (Z\alpha)^2$$

$$\gamma = \pm\sqrt{k^2 - (Z\alpha)^2}.$$

But we have $k = j + \frac{1}{2}$. Then

$$\gamma = \pm\sqrt{(j + \frac{1}{2})^2 - Z^2\alpha^2}. \tag{3.1.6}$$

Since the wave function has to be normalizable we must choose the positive sign for γ. For the negative solution $\gamma = |\gamma|$, it follows that $u_1^2 + u_2^2 \sim r^{-2|\gamma|}$ near the $r = 0$, which

would yield a divergent integral for the norm if $|\gamma| \leq \frac{1}{2}$. In-order to solve Eq. (3.1.2) we make the following substitutions:

$$\rho = 2\lambda r \ , \ \lambda = \frac{\left(m_0^2c^4 - E^2\right)^{1/2}}{\hbar c}. \tag{3.1.7}$$

Substituting $\frac{d\rho}{dr} = 2\lambda$ and $\frac{d}{dr} = 2\lambda\frac{d}{d\rho}$ and dividing by 2γ we obtain,

$$\begin{aligned}
\frac{du_1(\rho)}{d\rho} &= -\frac{ku_1(\rho)}{\rho} + \left[\frac{E + m_0c^2}{2\lambda\hbar c} + \frac{Z\alpha}{\rho}\right]u_2(\rho), \\
\frac{du_2(\rho)}{d\rho} &= \frac{ku_2(\rho)}{\gamma} - \left[\frac{E - m_0c^2}{2\lambda\hbar c} + \frac{Z\alpha}{\rho}\right]u_1(\rho).
\end{aligned} \tag{3.1.8}$$

Using this form of the equations we can get the behavior of $u_1(\rho)$ and $u_2(\rho)$ for $\rho \to \infty$, since neglecting the terms proportional to $1/\rho$ the differential equations of Eq. (3.1.8) gives as

$$\begin{aligned}
\frac{du_1(\rho)}{d\rho} &= \left(\frac{E + m_0c^2}{2\lambda\hbar c}\right)u_2(\rho), \\
\frac{du_2(\rho)}{d\rho} &= -\left(\frac{E - m_0c^2}{2\lambda\hbar c}\right)u_1(\rho).
\end{aligned} \tag{3.1.9}$$

Combining the second derivatives of this with Eq. (3.1.7), it follows immediately that

$$\begin{aligned}
\frac{d^2u_1(\rho)}{d\rho^2} &= -\left(\frac{E^2 - m_0^2c^4}{(2\hbar c\lambda)^2}\right)u_1(\rho), \\
\frac{d^2u_2(\rho)}{d\rho^2} &= -\left(\frac{E^2 - m_0^2c^4}{(2\hbar c\lambda)^2}\right)u_2(\rho).
\end{aligned}$$

But we have $\lambda^2 = \frac{(m_0^2c^4 - E^2)}{\hbar^2c^2}$. Then

$$\begin{aligned}
\frac{d^2u_1(\rho)}{d\rho^2} &= -\left(\frac{E^2 - m_0^2c^4}{(2\hbar c\lambda)^2}\right)u_1(\rho) = \frac{1}{4}u_1(\rho), \\
\frac{d^2u_2(\rho)}{d\rho^2} &= -\left(\frac{E^2 - m_0^2c^4}{(2\hbar c\lambda)^2}\right)u_2(\rho) = \frac{1}{4}u_2(\rho).
\end{aligned} \tag{3.1.10}$$

We can get two possible solutions with $u_1(\rho) = u_2(\rho) \sim e^{\pm\rho/2}$, but only the exponentially decreasing can be used since only this one is normalizable. This motivates the ansatz

$$\begin{aligned}
u_1(\rho) &= \left(m_0c^2 + E\right)^{1/2} e^{\rho/2}(\phi_1(\rho) + \phi_2(\rho)), \\
u_2(\rho) &= \left(m_0c^2 - E\right)^{1/2} e^{-\rho/2}(\phi_1(\rho) - \phi_2(\rho)).
\end{aligned} \tag{3.1.11}$$

inserting Eq. (3.1.11) in Eq. (3.1.8) gives:

$$(m_0c^2+E)^{1/2}e^{-\rho/2}\bigg[-\frac{1}{2}(\phi_1+\phi_2)+\frac{d\phi_1}{d\rho}+\frac{d\phi_2}{d\rho}\bigg]$$
$$=\frac{-k}{\rho}(m_0c^2+E)^{1/2}e^{-\rho/2}(\phi_1+\phi_2)+\bigg[\frac{E+m_0c^2}{2\hbar c\lambda}+\frac{Z\alpha}{\rho}\bigg](m_0c^2-E)^{\frac{1}{2}}\ e^{-\rho/2}(\phi_1-\phi_2),$$

$$(m_0c^2-E)^{\frac{1}{2}}\ e^{-\rho/2}\bigg[-\frac{1}{2}(\phi_1-\phi_2)+\frac{d\phi_1}{d\rho}-\frac{d\phi_2}{d\rho}\bigg]$$
$$=-\bigg[\frac{E-m_0c^2}{2\hbar c\lambda}+\frac{Z\alpha}{\rho}\bigg](m_0c^2+E)^{\frac{1}{2}}e^{-\rho/2}(\phi_1+\phi_2)$$
$$+\frac{k}{\rho}(m_0c^2-E)^{\frac{1}{2}}\ e^{-\rho/2}(\phi_1-\phi_2). \tag{3.1.12}$$

Dividing by $e^{-\rho/2}$ and furthermore the first equation by $(m_0c^2+E)^{\frac{1}{2}}$ and the second equation by $(m_0c^2-E)^{1/2}$ yields the result

$$-\frac{1}{2}(\phi_1+\phi_2)+\frac{d\phi_1}{d\rho}+\frac{d\phi_2}{d\rho}$$
$$=-\frac{k}{\rho}(\phi_1+\phi_2)+\bigg[\frac{E+m_0c^2}{2\hbar c\lambda}+\frac{Z\alpha}{\rho}\bigg]\frac{(m_0c^2-E)^{\frac{1}{2}}}{(m_0c^2+E)^{\frac{1}{2}}}(\phi_1-\phi_2),$$

$$-\frac{1}{2}(\phi_1-\phi_2)+\frac{d\phi_1}{d\rho}-\frac{d\phi_2}{d\rho}$$
$$=-\bigg[\frac{E-m_0c^2}{2\hbar c\lambda}+\frac{Z\alpha}{\rho}\bigg]\frac{(m_0c^2+E)^{\frac{1}{2}}}{(m_0c^2-E)^{\frac{1}{2}}}(\phi_1+\phi_2)+\frac{k}{\rho}(\phi_1-\phi_2). \tag{3.1.13}$$

On the other hand we have

$$\frac{(m_0c^2-E)^{\frac{1}{2}}}{(m_0c^2+E)^{\frac{1}{2}}}=\frac{m_0c^2-E}{\hbar c\lambda},$$

and

$$\frac{(m_0c^2+E)^{\frac{1}{2}}}{(m_0c^2-E)^{\frac{1}{2}}}=\frac{m_0c^2+E}{\hbar c\lambda}. \tag{3.1.14}$$

Therefore

$$-\frac{1}{2}(\phi_1+\phi_2)+\frac{d\phi_1}{d\rho}+\frac{d\phi_2}{d\rho}$$
$$=-\frac{k}{\rho}(\phi_1+\phi_2)+\bigg[\frac{E+m_0c^2}{2\hbar c\lambda}+\frac{Z\alpha}{\rho}\bigg]\frac{(m_0c^2-E)^{\frac{1}{2}}}{\hbar c\lambda}(\phi_1-\phi_2),$$

$$-\frac{1}{2}(\phi_1-\phi_2)+\frac{d\phi_1}{d\rho}-\frac{d\phi_2}{d\rho}$$
$$=-\left[\frac{E-m_0c^2}{2\hbar c\lambda}+\frac{Z\alpha}{\rho}\right]\frac{(m_0c^2+E)^{\frac{1}{2}}}{\hbar c\lambda}(\phi_1+\phi_2)+\frac{k}{\rho}(\phi_1-\phi_2). \tag{3.1.15}$$

Adding both equations of Eq. (3.1.15) yields

$$-\phi_1+2\frac{d\phi_1}{d\rho}$$
$$=-\frac{2k}{\rho}\phi_2+\phi_1+\frac{Z\alpha}{\rho}(\frac{m_0c^2-E}{\hbar c\lambda})(\phi_1-\phi_2)$$
$$-\frac{Z\alpha}{\rho}(\frac{m_0c^2+E}{\hbar c\lambda})(\phi_1+\phi_2) \tag{3.1.16}$$

Whereas by subtracting them we get

$$-\phi_2+2\frac{d\phi_2}{d\rho}$$
$$=-\frac{2k}{\rho}\phi_1-\phi_2+\frac{Z\alpha}{\rho}(\frac{m_0c^2-E}{\hbar c\lambda})(\phi_1-\phi_2)$$
$$+\frac{Z\alpha}{\rho}(\frac{m_0c^2+E}{\hbar c\lambda})(\phi_1+\phi_2) \tag{3.1.17}$$

Summarizing all this yields

$$\frac{d\phi_1}{d\rho}=\left(1-\frac{Z\alpha E}{\hbar c\lambda\rho}\right)\phi_1-\left(\frac{k}{\rho}+\frac{Z\alpha m_0c^2}{\hbar c\lambda\rho}\right)\phi_2,$$
$$\frac{d\phi_2}{d\rho}=\left(-\frac{k}{\rho}+\frac{Z\alpha m_0c^2}{\hbar c\lambda\rho}\right)\phi_1+\frac{Z\alpha E}{\hbar c\lambda\rho}\phi_2. \tag{3.1.18}$$

In order to find the solutions for ϕ_1 and ϕ_2 we make the ansatz of a power series expansion. Separating out of a factor ρ^γ, which describes the behavior of the solution for $\rho\to 0$, we write

$$\phi_1=\rho^\gamma\sum_{m=0}^{\infty}\alpha_m\rho^m,$$
$$\phi_2=\rho^\gamma\sum_{m=0}^{\infty}\beta_m\rho^m. \tag{3.1.19}$$

Inserting these in Eq. (3.1.18) yields

$$\sum(m+\gamma)\alpha_m\rho^{m+\gamma-1}$$
$$=\sum\alpha_m\rho^{m+\gamma}-\frac{Z\alpha E}{\hbar c\lambda}\sum\alpha_m\rho^{m+\gamma-1}-\left(k+\frac{Z\alpha m_0c^2}{\hbar c\lambda}\right)\sum\beta_m\rho^{m+\gamma-1},$$

$$\sum \beta_m(m+\gamma)\rho^{m+\gamma-1}$$
$$= \left(-k + \frac{Z\alpha m_0 c^2}{\hbar c\lambda} \right) \sum \alpha_m \rho^{m+\gamma-1} + \frac{Z\alpha E}{\hbar c\lambda} \sum \beta_m \rho^{m+\gamma-1}. \tag{3.1.20}$$

Comparing the coefficients, we get

$$\alpha_m(m+\gamma) = \alpha_{m-1} - \frac{Z\alpha E}{\hbar c\lambda}\alpha_m - \left(k + \frac{Z\alpha m_0 c^2}{\hbar c\lambda}\right)\beta_m,$$

$$\beta_m(m+\gamma) = \left(-k + \frac{Z\alpha m_0 c^2}{\hbar c\lambda} \right)\alpha_m + \frac{Z\alpha E}{\hbar c\lambda}\beta_m. \tag{3.1.21}$$

From the second equation of Eq. (3.1.21) it follows that

$$\frac{\beta_m}{\alpha_m} = \frac{-k + Z\alpha m_0 c^2/\hbar c\lambda}{m+\gamma - Z\alpha E/\hbar c\lambda} = \frac{k - Z\alpha m_0 c^2/\hbar c\lambda}{n' - m}, \tag{3.1.22}$$

with

$$n' = \frac{Z\alpha E}{\hbar c\lambda} - \gamma \tag{3.1.23}$$

For $m = 0$ we get

$$\frac{\beta_0}{\alpha_0} = \frac{k - Z\alpha m_0 c^2/\hbar c\lambda}{n'} = \frac{k - (n'+\gamma)m_0 c^2/E}{n'}. \tag{3.1.24}$$

Now inserting the result Eq. (3.1.22) in the first equation of Eq. (3.1.21) yields

$$\alpha_m \left[m + \gamma + \frac{Z\alpha E}{\hbar c\lambda} + \left(k + \frac{Z\alpha m_0 c^2}{\hbar c\lambda}\right)\left(\frac{k - Z\alpha m_0 c^2/\hbar c\lambda}{(n'-m)}\right)\right] = \alpha_{m-1}, \tag{3.1.25}$$

or

$$\alpha_m \left[\left(m + \gamma + \frac{Z\alpha E}{\hbar c\lambda}\right)(n'-m) + k^2 - \frac{Z^2\alpha^2 m_0^2 c^4}{\hbar^2 c^2 \lambda^2} = \alpha_{m-1}(n'-m). \right. \tag{3.1.26}$$

We calculate both brackets on the left hand side of Eq. (59)

$$\left(m + \gamma + \frac{Z\alpha E}{\hbar c\lambda}\right)\left(\frac{Z\alpha E}{\hbar c\lambda} - \gamma - m\right) = -2m\gamma - m^2 - \gamma^2 + \left(\frac{Z\alpha E}{\hbar c\lambda}\right)^2, \tag{3.1.27}$$

with $\gamma^2 = k^2 - (Z\alpha)^2$ and it follows that

$$\alpha_m \left[-m(2\gamma + m) + (Z\alpha)^2 + \left(\frac{Z\alpha E}{\hbar c\lambda}\right)^2 - \left(\frac{Z\alpha m_0 c^2}{\hbar c\lambda}\right)^2 \right]$$

$$= \alpha_{m-1}(n' - m), \tag{3.1.28}$$

which can be further summarized as

$$\begin{aligned} \alpha_m &= -\frac{(n'-m)}{m(2\gamma+m)}\alpha_{m-1} = (-1)^m \frac{(n'-1)...(n'-m)}{m!(2\gamma+1)...(2\gamma+m)}\alpha_0 \\ &= \frac{(1-n')(2-n')..(m-n')}{m!(2\gamma+1)...(2\gamma+m)}\alpha_0. \end{aligned} \tag{3.1.29}$$

According to Eq. (3.1.22) β_m is found to be

$$\beta_m = \frac{(k - Z\alpha m_0 c^2)}{(n'-m)\hbar c\lambda} \frac{(-1)^m (n'-1)...(n'-m)}{m!(2\gamma+1)...(2\gamma+m)}\alpha_0. \tag{3.1.30}$$

Using Eq. (3.1.24) this yields

$$\beta_m = (-1)^m \frac{n'(n'-1)...(n'-m+1)}{m!(2\gamma+1)...(2\gamma+m)}\beta_0. \tag{3.1.31}$$

This power series turns out to be the confluent hyper-geometric function

$$F(a,b;x) = 1 + \frac{a}{b}x + \frac{a(a+1)}{b(b+1)}\frac{x^2}{2!} + ... \quad . \tag{3.1.32}$$

We thus find that

$$\begin{aligned} \phi_1 &= \alpha_0 \rho^\gamma F(1-n', 2\gamma+1; \rho), \\ \phi_2 &= \beta_0 \rho^\gamma F(-n', 2\gamma+1; \rho) \\ &= \left(\frac{k - Z\alpha m_0 c^2/\hbar c\lambda}{n'}\right)\alpha_0 \rho^\gamma F(-n', 2\gamma+1; \rho). \end{aligned} \tag{3.1.33}$$

In order the wave functions remain normalizable we must require that the series for ϕ_1 and ϕ_2 terminate. Thus the hyper-geometric functions have to be simple polynomials. This can only be achieved if n' is a non-negative integer, i.e. $n' = 0, 1, 2, ...$

We defined a principal quantum number

$$n = n' + |k| = n' + j + \frac{1}{2}\ ,\ n = 1, 2, 3, ... \quad . \tag{3.1.34}$$

With this we can calculate the energy eigenvalue from Eq.(3.1.23) as,

$$\frac{Z\alpha E}{(m_0^2 c^4 - E^2)^{1/2}} = n' + \gamma = n - j - \frac{1}{2} + \gamma \tag{3.1.35}$$

and consequently

$$\left[(Z\alpha)^2 + (n - j - \frac{1}{2} + \gamma)^2\right] E^2 = m_0^2 c^4 (n - j - \frac{1}{2} + \gamma)^2.$$

Then

$$E^2 = \frac{m_0^2 c^4 (n - j - \frac{1}{2} + \gamma)^2}{(Z\alpha)^2 + (n - j - \frac{1}{2} + \gamma)^2}$$

$$\Rightarrow \; E = \pm m_0 c^2 \left[1 + \frac{(Z\alpha)^2}{[n - j - \frac{1}{2} + [(j + \frac{1}{2})^2 - (Z\alpha)^2]^{\frac{1}{2}}]^2}\right]^{-\frac{1}{2}},$$

$$\begin{aligned} n \quad &= 1, 2, 3... \quad , \\ k &= \pm(j + \frac{1}{2}) = \pm 1, \pm 2, \pm 3, ... \qquad . \end{aligned} \tag{3.1.36}$$

The negative sign in Eq. (3.1.36) must be excluded because, for positive charge nuclei ($Z\alpha > 0$), negative energies E do not fulfill the original equation Eq. (3.1.35), since its rhs is positive. We therefore write the negative sign in Eq. (3.1.36) in parenthesis, and we thus obtain the Sommerfeld fine-structure formula for the energy eigenvalues of electrons in atom with coulomb potential and point nuclei.

3.2 The wave function at the diving point

The Dirac wave function at the diving point can be determined at $E = -m_0$. In this section we will obtain the second order differential equation of wave function u_1, and the modified Bessel's differential equation of wave function u_1.

3.2.1 The second order differential equation of wave function u_1

The system of two coupled ordinary differential equation can be written as differential equation of second order of the wave function u_1 by eliminating the wave function u_2. In Eq.(2.0.35) we have already obtained the system of two coupled ordinary differential

equation of the wave function u_1 and u_2 in the first order ($\hbar = c = 1$) as

$$\begin{aligned} \frac{du_1(r)}{dr} &= -\frac{k}{r}u_1(r) + [E + m_0 - V(r)]u_2(r), \\ \frac{du_2(r)}{dr} &= \frac{k}{r}u_2(r) - [E - m_0 - V(r)]u_1(r). \end{aligned} \tag{3.2.1}$$

Now differentiate the first equations of Eq. (3.2.1) with respect to r, which gives

$$u_1'' = \frac{k}{r^2}u_1 - \frac{k}{r}u_1' - V'u_2 + (E + m_0 - V)u_2'. \tag{3.2.2}$$

Again we express the first equations of Eq. (3.2.1) as

$$u_2 = \frac{u_1' + \frac{k}{r}u_1}{E + m_0 - V}. \tag{3.2.3}$$

Inserting Eq. (3.2.3) in the second equation of (3.2.1) gives

$$u_2' = -(E - m_0 - V)u_1 + \frac{\frac{k}{r}u_1' + \frac{k^2}{r^2}u_1}{E + m_0 - V}. \tag{3.2.4}$$

Then by inserting Eqs. (3.2.3) and (3.2.4) in Eq. (3.2.2) in terms of u_2 and u_2' respectively we get

$$u_1'' + \frac{V'}{E + m_0 - V}u_1' + \left[(E - V)^2 - m_0^2 - \frac{k(k+1)}{r^2} + \frac{k}{r}\frac{V'}{E + m_0 - V}\right]u_1 = 0 \tag{3.2.5}$$

which is the second order differential equation of the system of two coupled ordinary differential equation for wave function u_1.

3.2.2 The modified Bessel's differential equation of wave function u_1

The coulomb potential is given by $V(r) = -Z\alpha/r$. Now we differentiate with respect to r which gives, $V'(r) = Z\alpha/r^2$. By inserting the value of V and V' at the diving point where $E = -m_0$, Eq. (3.2.5) is reduced to

$$u_1'' + \frac{1}{r}u_1' - \left(\frac{2m_0 Z\alpha}{r} - \frac{(Z\alpha)^2 - k^2}{r^2}\right)u_1 = 0. \tag{3.2.6}$$

Let $\rho^2 = 8m_0 Z\alpha r$, then

$$\frac{d}{dr} = \frac{4m_0 Z\alpha}{\rho}\frac{d}{d\rho},$$
$$\frac{d^2}{dr^2} = \frac{(4m_0 Z\alpha)^2}{\rho^2}\Big(-\frac{1}{\rho}\frac{d}{d\rho} + \frac{d^2}{d\rho^2}\Big). \tag{3.2.7}$$

Inserting Eq. (3.2.7) in Eq. (3.2.6), it gives

$$\frac{(4m_0 Z\alpha)^2}{\rho^2}\Big(-\frac{1}{\rho}\frac{d}{d\rho} + \frac{d^2}{d\rho^2}\Big)u_1 + \frac{1}{r}\frac{(4m_0 Z\alpha)}{\rho}\frac{d}{d\rho}u_1$$
$$-\Big(\frac{2m_0 Z\alpha}{r} - \frac{(Z\alpha)^2 - k^2}{r^2}\Big)u_1 = 0.$$

$$\frac{(4m_0 Z\alpha)^2}{\rho^2}\Big(-\frac{1}{\rho}\frac{d}{d\rho}u_1 + \frac{d^2}{d\rho^2}u_1\Big) + \frac{1}{r}\frac{(4m_0 Z\alpha)}{\rho}\frac{d}{d\rho}u_1$$
$$-\Big(\frac{2m_0 Z\alpha}{r} - \frac{(Z\alpha)^2 - k^2}{r^2}\Big)u_1 = 0.$$

But $r = \rho^2/8m_0 Z\alpha$, then

$$\frac{(4m_0 Z\alpha)^2}{\rho^2}\frac{d^2}{d\rho^2}u_1 - \frac{(4m_0 Z\alpha)^2}{\rho^2}\frac{d}{\rho d\rho}u_1 - \Big\{(\tfrac{2m_0 Z\alpha}{\rho^2})(8m_0 Z\alpha) - (\tfrac{(2\alpha)^2 - k^2}{\rho^4})(8m_0 Z\alpha)^2\Big\}u_1 = 0.$$

Now multiplying by $\rho^2/(4m_0 Z\alpha)^2$ leads to

$$\frac{d^2}{d\rho^2}u_1 + \frac{1}{\rho}\frac{d}{d\rho}u_1 - \Big\{1 - \tfrac{4[(Z\alpha)^2 - k^2]}{\rho^2}\Big\}u_1 = 0. \tag{3.2.8}$$

$$f'' + \frac{1}{\rho}f' - \Big(1 + \frac{\mu^2}{\rho^2}\Big)f = 0. \tag{3.2.9}$$

This is just the differential equation obeyed by the modified Bessel functions. This differential equation is solved by the linearly independent solutions $k_\mu(\rho)$ and $I_\mu\ (\rho)$. The function $I_\mu\ (\rho)$ is to be rejected since it increases exponentially at infinity. Therefore the normalizable solution of the Dirac equation at the critical point reads

$$u_1(r) = c k_{iv}\big(\sqrt{8m_0 Z\alpha r}\big). \tag{3.2.10}$$

The index of the modified Bessel function (Mc Donald function) is purely imaginary in the case $Z\alpha > |k|$, being given by

$$\nu = 2\sqrt{(Z\alpha)^2 - \kappa^2}. \tag{3.2.11}$$

The lower component of the wave function follows from Eq. (3.2.3)

$$u_2(r) = \frac{c}{Z\alpha}\left[\frac{1}{2}\sqrt{8m_0Z\alpha r}K'_{i\nu}(\sqrt{8m_0Z\alpha r}) + \kappa K_{i\nu}(\sqrt{8m_0Z\alpha r})\right]. \tag{3.2.12}$$

where $K'_{i\nu}$ denotes the derivative of the Bessel function with respect to its argument and the first equations of Eq. (3.2.7) has been used. The "critical wave function"decays exponentially as a function of $\sqrt{r}$ for large values of r, since

$$K_{i\nu}(z) \to \sqrt{\frac{\pi}{2z}}e^{-z} \quad for \quad z \to \infty. \tag{3.2.13}$$

The limit $r \to 0$ is more involved.

$$K_{i\nu}(z) \to \sqrt{\frac{\pi}{\nu sinh\pi\nu}}sin\left(v\ln\frac{2}{z} + arg\Gamma(1+i\nu)\right). \tag{3.2.14}$$

3.3 The Sommerfeld fine-structure formula and the classification of the electron levels

For the electron eigenvalues in a coulomb potential, we have derived

$$E = +m_0c^2\left[1 + \frac{(Z\alpha)^2}{[n-j-\frac{1}{2}+[(j+\frac{1}{2})^2-(Z\alpha)^2]^{\frac{1}{2}}]^2}\right]^{-\frac{1}{2}}, \tag{3.3.1}$$

where

$n' = n - j - \frac{1}{2} = n - |k|$,

$n = 1, 2, 3, ...$

$j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}...$.

The energy eigenvalues thus only depend on the principal quantum number n, $|k|$ and Z. For a vanishing potential ($Z = 0$) the energy eigenvalue is $+m_0C^2$. The bound electron states thus adjoin the continuum of positive energy beginning at $+m_0c^2$. This is plausible because, due to a "switching on of the potential", that is, due to a continuous increase of the coupling strength Z_α from $Z_\alpha = 0$, electron states from the positive energy continuum can be"pulled"into the energy gap between $+m_0c^2$ and -m_0c^2, thus becoming

bound states. The limit of ionization of an electronic atom is obviously m_0c^2, and the ionization energy of an electron in the state n_j is

$$E_{ioniz} = m_0c^2\left\{1 - \left[1 + \frac{(Z\alpha)^2}{[n - j - \frac{1}{2} + [(j+\frac{1}{2})^2 - (Z\alpha)^2]^{\frac{1}{2}}]^2}\right]^{-\frac{1}{2}}\right\}$$

$$\approx m_0c^2(Z\alpha)^2\left\{\frac{1}{2n^2} + \frac{(Z\alpha)^2}{2n^3}\left(\frac{1}{|k|} - \frac{3}{4n}\right)\right\}, \tag{3.3.2}$$

which is equal to the negative binding energy, i.e. $E_{bind} = -E_{ioniz}$. We draw attention to the existence of bound states even for negative nuclear charge $Z\alpha < 0$ with energies corresponding to the negative of the solutions for $Z\alpha > 0$.

For the states with $j = \frac{1}{2}$, energy values can be calculated up to $Z\alpha \leq 1$, i.e. up to $Z \sim 137$; for $j = \frac{1}{2}$, $n = 1$. Then

$$E = m_0c^2\left[1 + \frac{(z\alpha)^2}{1 - Z^2\alpha^2}\right]^{-\frac{1}{2}} = m_0c^2\sqrt{1 - Z^2\alpha^2}.$$

For $Z\alpha = 1$ yields $E = 0$ or $E_{bind} = E - m_0c^2 = -m_0c^2$. With increasing Z the absolute value of the binding energy also increases. The slope dE/dZ approaches infinity for this $1s_{\frac{1}{2}}$ state ($n = 1$, $l = 0$, $j = 1/2$) at $Z\alpha = 1$, while for $Z\alpha > j + \frac{1}{2}$ the energy becomes imaginary. Thus it seems that there exist no bound $ns_{\frac{1}{2}}$ or $np_{\frac{1}{2}}$ states for point nuclei with charge greater than $Z = \frac{1}{\alpha} = 137$. This strange result can be understood in connection with the supercritical phenomena as a collapse of the vacuum; a new, fundamental process.

To calculate actual numbers, we replace m_0c^2 by the electron's rest mass $m_0c^2 = 0.5110041MeV$. For $n' = 0$ the confluent series terminates only for $k < 0$. For $k > 0$ they diverge even for $n' = 0$. It thus follows that

$$n' = \begin{cases} 0, 1, 2, ... \; for \; k < 0, \\ 1, 2, 3, ... \; for \; k > 0. \end{cases} \tag{3.3.3}$$

For $Z\alpha \ll 1$ the energy formula can be expanded as,

$$\frac{E - m_0c^2}{m_0c^2} = -(Z\alpha)^2\left\{\frac{1}{2n^2} + \frac{(Z\alpha)^2}{2n^3}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right)\right\}. \tag{3.3.4}$$

The first term in Eq. (3.3.4) represents the Bohr formula for the energy levels of the atom calculated according to the Schrodinger equation. Accordingly, relativistic corrections for the energy levels in a Coulomb field are of the order $(Z\alpha)^2$. These corrections are only significant for small principal quantum numbers and in heavy nuclei. Furthermore we note that the relativistic wave functions $f(r)$ and $g(r)$ show for $|k| = 1$ a weak (but quadratically integrable) divergence at the origin $r = 0$, in contrast to the non relativistic case. The quantum number k takes the values $k = \pm 1, \pm 2, ...$, and the principal quantum number n the values $n = 1, 2, ...,$. We recall that for $n' = 0$ the quantum number k must be positive and thus from Eq. (3.1.34), we have $k = n$ and consequently, $l = n - 1$ and $j = n - 1/2$. The states are classified in complete accordance to the levels of the hydrogen atom ($Z = 1$), as summarized in detail in the following table 3.1. for the values of quantum numbers k, j, n' and l for the given value of the principal quantum number n, where the notation part nlj which refers n is the principal quantum number, l is orbital quantum number ($l = 0(s)$, $1(p)$, $2(d)$, $3(f)$,...) and the values of j and n' are calculated as $j = l + 1/2$ and $n' = n - j - 1/2$. Table 3.2 shows the binding energy for the $1s_1/2$ electron as a function of Z. The situation is illustrated in Fig.3.1.

Figure 3.1 displays the result of numerical calculations for the energies of several bound states as a function of nuclear charge Z. The energy levels descend progressively with increasing Z. The energy of the lowest state ($1s$, $k = 1$) becomes negative when $Z > 150$. The $1s$ level finally reaches the value $E_{1s} = -m_0c^2$ at a critical charge $Z_{cr}^{1s} \simeq 173$, and the Sommerfeld energies of the states with $k = -1(ns_{1/2})$ and $k = +1(np_{1/2})$ break off with a vertical tangent at $z\alpha = 1$ (dotted curve). The same happens for the $2p_{1/2}$ state with $k = +1$ at $Z_{cr}^{2p_{1/2}} \simeq 185$, whereas higher states reach the lower continuum $E = -m_0c^2$ at much larger critical charges Z_{cr}.

$Notation$	n	l	j	n'	k	E_{bind}/eV
$1s_{1/2}$	1	0	1/2	0	-1	-13.606
$2s_{1/2}$	2	0	1/2	1	-1	-3.402
$2p_{1/2}$	2	1	1/2	1	1	-3.402
$2p_{3/2}$	2	1	3/2	0	-2	-3.401
$3s_{1/2}$	3	0	1/2	2	-1	-1.512
$3p_{1/2}$	3	1	1/2	2	1	-1.512
$3p_{3/2}$	3	1	3/2	1	-2	-1.512
$3d_{3/2}$	3	2	3/2	1	2	-1.512
$3d_{5/2}$	3	2	5/2	0	-3	-1.512
$4s_{1/2}$	4	0	1/2	3	-1	-0.850
$4p_{1/2}$	4	1	1/2	3	1	-0.850
$4p_{3/2}$	4	1	3/2	2	-2	-0.850
$4d_{3/2}$	4	2	3/2	2	2	-0.850
$4d_{5/2}$	4	2	5/2	1	-3	-0.850
$4f_{5/2}$	4	3	5/2	1	3	-0.850
$4f_{7/2}$	4	3	7/2	0	-4	-0.850

Table 3.1: The classification of bound states of the electron according to the Dirac equation for $Z = 1$ (hydrogen atom)

Z	E_{bind}/eV	Z	E_{bind}/eV
10	-1362	80	-96117
20	-5472	90	-125657
30	-12396	100	-161615
40	-22254	110	-206256
50	-35229	120	-264246
60	-51585	130	-349368
70	-71699	137	-499288

Table 3.2: Binding energies for $1s_{1/2}$ electrons as a function of Z according to the Sommerfeld fine-structure formula

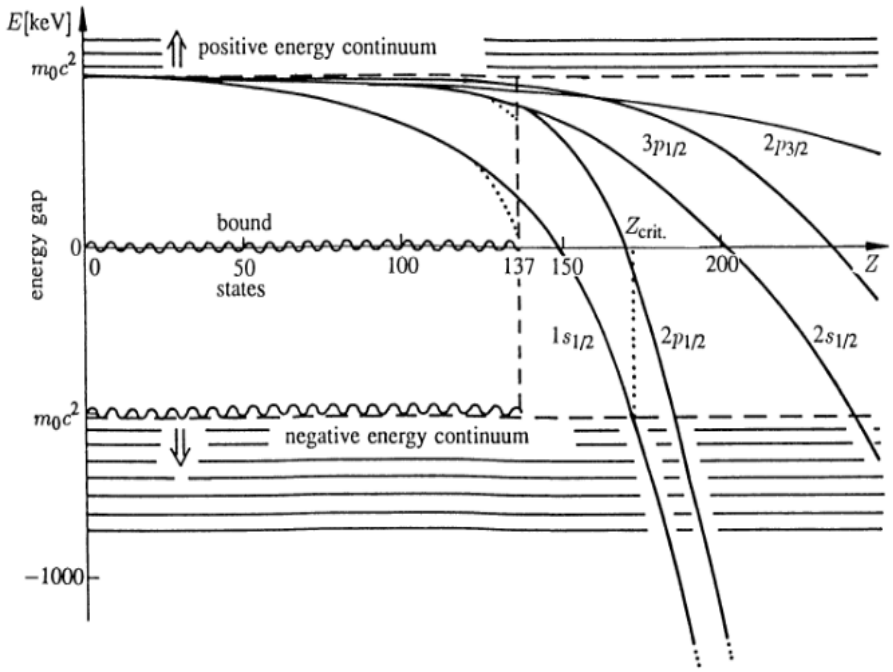

Figure 3.1: The lowest bound states of the Dirac equation for atoms with nuclear charge Z

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Chapter 4

Fano's Formalism for the Description of Resonances

It is a common problem in applications of quantum mechanics that an initially stable system becomes unstable and can decay if a small perturbation is switched on. Mathematically speaking one starts with a system characterized by a Hamiltonian H_0 which possesses at least one discrete and normalizable eigenstate ϕ_0 with energy E_0 ,i.e.

$$H_0\phi_0 = E_0\phi_0. \tag{4.0.1}$$

Furthermore, H_0 is assumed to have a continuous spectrum, i.e.

$$H_0\psi_E = E\psi_E, \tag{4.0.2}$$

for a certain range of energy values. (In the case of spontaneous positron production, which is of interest here, this range is $-\infty < E < -m_0c^2$). We require that the wave functions ψ_E asymptotically ($r \to \infty$) are stationary standing waves. The following orthonormality conditions holds:

$$\begin{aligned} &\langle\phi_0|\phi_0\rangle = 1, \\ &\langle\psi_E|\phi_0\rangle = 0, \\ &\langle\psi_{E'}|\psi_E\rangle = \delta(E' - E). \end{aligned} \tag{4.0.3}$$

The continuum thus is normalized "to a delta function". An additional interaction is added now, in the form of a perturbation potential V':

$$H = H_0 + V'. \tag{4.0.4}$$

Here it can happen that the discrete state ϕ_0 is lost under the influence of the interaction. It amalgamates with the continuum (it is "embedded" into it) which is now described by the equation

$$H\Psi_E = E\Psi_E, \tag{4.0.5}$$

again with the normalization

$$\langle \Psi_{E'} | \Psi_E \rangle = \delta(E' - E). \tag{4.0.6}$$

If this occurs it will be no longer possible to keep the system in a localized stationary state. Physically, the following happens: The previously stable system decays by emission of one of its constituents (since a continuous spectrum is always related to a motion to infinity). In a time-dependent description it can actually be shown that the probability to encounter the state ϕ_0 decreases to zero exponentially in time after the perturbation V' has been switched on.

From the point of view of quantum mechanical scattering theory the presence of a previously bound state ϕ_0 manifests as a resonance with its well known signatures: The scattering cross section grows in the vicinity of the resonance energy, the scattering phase varies rapidly as a function of E, the density of the wave function $|\Psi_E(x)|^2$ is strongly enhanced at small distances. We now want to examine the properties of the solution of Eq. (4.0.5) making use of the solutions of the unperturbed problem Eqs. (4.0.1) and (4.0.2). To achieve this we employ a method that was developed by U. Fano for the case of autoionisation of excited states in atomic physics.

The new continuum wave function is expanded as

$$\Psi_E(x) = a(E)\phi_0(x) + \int dE' h_{E'}(E)\psi_{E'}(x), \tag{4.0.7}$$

the integral extends over the entire range of the continuum. Assumed that Ψ_E is in that Hilbert space that is spanned by the set $\left\{\phi_0, \psi_{E'}\right\}$. If the spectrum of H_0 does contain additional (discrete or continuous) parts, these states could also be admixed by the action of V'.

The expansion coefficients are given by

$$\begin{aligned} a(E) &= \langle\phi_0|\Psi_E\rangle, \\ h_{E'}(E) &= \langle\psi_{E'}|\Psi_E\rangle. \end{aligned} \tag{4.0.8}$$

but this does not help us much as long as Ψ_E is unknown. We now use Eq. (4.0.5) and project onto $\langle\phi_0|$ and $\langle\psi_{E'}|$. Now using Eqs. (4.0.3) and (4.0.7) the system of equations becomes

$$\begin{aligned} (E - E_0 - \Delta E)a(E) &= \int dE' V^*_{E'} h_{E'}(E) \\ (E - E')h_{E'}(E) &= V_{E'}a(E) + \int dE'' U_{E'E''} h_{E''}(E) \end{aligned} \tag{4.0.9}$$

The abbreviations used are

$$\begin{aligned} E_0 + \Delta E \quad &= \langle\phi_0|H|\phi_0\rangle \\ &= \langle\phi_0|H_0|\phi_0\rangle + \langle\phi_0|V'|\phi_0\rangle, \\ V_E &= \langle\psi_E|H|\phi_0\rangle = \langle\psi_E|V'|\phi_0\rangle, \\ U_{E'E''} &= \langle\psi_{E'}|V'|\psi_{E''}\rangle. \end{aligned} \tag{4.0.10}$$

E_0 is the original energy of the bound state of H_0. The expectation value ΔE of $H - H_0 = V'$ in this state is equal to the energy shift in first-order perturbation theory. The matrix element V'_E specifies how strongly the bound state couples to the continuum, and $U_{E'E''}$ describes the mixing among the continuum states. Additionally, there is the normalization condition Eq. (4.0.6), namely

$$a^*(E)a(E') + \int dE'' h^*_{E''}(E) h_{E''}(E') = \delta(E - E'). \tag{4.0.11}$$

An analytic solution may be found if the coupling term $U_{E'E''}$ in the second equations of Eq. Eq. (4.0.9) of the second term is neglected, i.e.

$$\int dE'' U_{E'E''} h_{E''}(E) \simeq 0. \tag{4.0.12}$$

This could in principle be achieved by a unitary transformation the ψ_E,

$$\chi E = \int dE' M_{EE'} \psi E', \tag{4.0.13}$$

with suitably chosen coefficients $M_{EE'}$, such that $\langle \chi E' | H | \chi E \rangle$ becomes diagonal. On the other hand the distortion of the continuum by $UE'E''$ does not change the solution of the problem qualitatively so that we shall use the approximation Eq. (4.0.12) in the following. In order to solve the system of Eqs. (4.0.9) and (4.0.11) we split the expansion coefficient $h_{E'}(E)$ into

$$h_{E'}(E) = C_{E'}(E) a(E). \tag{4.0.14}$$

In this way $a(E)$ is eliminated from the two equations of Eq. (4.0.9), i.e.

$$\begin{aligned} E - E_0 - \Delta E &= \int dE' V^*_{E'} C_{E'}(E), \\ (E - E') C_{E'}(E) &= V_{E'}. \end{aligned} \tag{4.0.15}$$

The second equations of Eq. (4.0.15) is written as

$$C_{E'}(E) = \frac{V_{E'}}{E - E'}. \tag{4.0.16}$$

Here the question arises how to treat the pole at $E = E'$. In the treatment of scattering problems usually such poles are shifted by a small imaginary part into the complex plane and the requirement of causality is used. Following Fano we want to go a different way, however, that is adapted to the chosen boundary conditions (standing waves). Therefore we replace Eq. (4.0.16) by

$$C_{E'}(E) = P \frac{V_{E'}}{E - E'} + g(E) V_E \delta(E - E'), \tag{4.0.17}$$

where P means that Cauchy's principal value is to be taken in the energy integration. $C_{E'}(E)$ Eq. (4.0.17) solves the second equations of Eq. (4.0.15) for any arbitrary function $g(E)$ because of $x\delta(x) = 0$. The unknown function $g(E)$ may now be determined by inserting in the first equations of Eq. (4.0.15),

$$E - E_0 - \Delta E = P \int dE' \frac{|V_{E'}|^2}{E - E'} + g(E)|V_E|^2, \tag{4.0.18}$$

Or

$$g(E) = \frac{1}{|V_E|^2}[E - E_0 - \Delta E - F(E)], \tag{4.0.19}$$

where

$$F(E) = P \int dE' \frac{|V_{E'}|^2}{E - E'}. \tag{4.0.20}$$

$a(E)$ has to be determined from the normalization condition Eq. (4.0.11). Now insert Eq. (4.0.19) in Eq. (4.0.17) we get

$$\begin{aligned} a^*(E)a(E')\Bigg[1 + \int dE'' V^*_{E''}\left(P\frac{1}{E - E''} + g(E)\delta(E - E'')\right) \\ \times\left((P\frac{1}{E' - E''} + g(E')\delta(E' - E'')\right)V_{E''}\Bigg] = \delta(E - E'), \end{aligned} \tag{4.0.21}$$

Or

$$\begin{aligned} a^*(E)a(E')\Bigg(1 + \int dE''|V_{E''}|^2 P\frac{1}{E - E''}P\frac{1}{E' - E''} \\ +g(E')|V_{E'}|^2 P\frac{1}{E - E'} + g(E)|V_E|^2 P\frac{1}{E' - E} \\ +g^2(E)|V_E|^2\delta(E - E')\Bigg) = \delta(E - E'), \end{aligned} \tag{4.0.22}$$

Let us use the following properties of the delta function

$$\delta(E - E'')\delta(E' - E'') = \delta(E - E')\delta(E - E'') \tag{4.0.23}$$

$$\int dE' f(E')\delta(E - E') = f(E) \tag{4.0.24}$$

The product of the two principle-value factors in Eq. (4.0.22) is troublesome if the poles coincide, i.e. $E = E'$. And we have

$$\begin{aligned} & P\frac{1}{E-E''}P\frac{1}{E'-E''} \\ & = -P\frac{1}{E-E'}\left(P\frac{1}{E-E''} - P\frac{1}{E'-E''}\right) + \pi^2\delta(E-E'')\delta(E'-E''). \end{aligned} \tag{4.0.25}$$

holds for such an expression. Inserting this in Eq. (4.0.22) together with definition Eq. (4.0.20) yields

$$\begin{aligned} & a^*(E)a(E')\Bigg[1 - P\frac{1}{E-E'}(F(E)-F(E')) \\ & +g(E')|V_E'|^2 P\frac{1}{E-E'} - g(E)|V_E|^2 P\frac{1}{E-E'} \\ & +\pi^2|V_E|^2\delta(E-E') + g^2(E)|V_E|^2\delta(E-E')\Bigg] = \delta(E-E'). \end{aligned} \tag{4.0.26}$$

Now lets collect the principal-value terms

$$\begin{aligned} & -P\frac{1}{E-E'}\left[\left(F(E)+g(E)|V_E|^2\right) - \left(F(E')+g(E')|V_{E'}|^2\right)\right] \\ & = -P\frac{1}{E-E'}(E-E') = -1. \end{aligned}$$

Where Eq. (4.0.19) has been used for $g(E)$. Obviously all terms without the factor $\delta(E-E)$ cancel out in Eq. (4.0.26) such that a consistent equation remains

$$a^*(E)a(E')\left(\pi^2|V_E|^2 + g^2(E)|V_E|^2\right)\delta(E-E') = \delta(E-E'), \tag{4.0.27}$$

or

$$\begin{aligned} |a(E)|^2 = \quad & \frac{1}{|V_E|^2(g^2(E)+\pi^2)} = \frac{|V_E|^2}{(E-E_0-\Delta E-F(E))^2+\pi^2|V_E|^4} \\ & = \frac{\Gamma_E/2\pi}{(E-E_r)^2+\Gamma_E^2/4}, \end{aligned} \tag{4.0.28}$$

where

$$\begin{aligned} \Gamma_E &= 2\pi|V_E|^2, \\ E_r &= E_0 + \Delta E + F(E). \end{aligned} \tag{4.0.29}$$

The expansion coefficient $a(E)$ can be written as

$$a(E) = \frac{1}{V_E\sqrt{g^2(E)+\pi^2}} = \frac{V_E^*}{\sqrt{(E-E_r)^2+\Gamma_E^2/4}}. \tag{4.0.30}$$

If the matrix element V_E is real we obtain

$$a(E) = \sqrt{\frac{\Gamma_E/2\pi}{(E-E_r)^2+\Gamma_E^2/4}}. \tag{4.0.31}$$

Because of Eqs. (4.0.14) and (4.0.7)

$$h_{E'}(E) = \frac{V_E^*}{\sqrt{(E-E_r)^2+\Gamma_E^2/4}}\left(P\frac{V_{E'}}{E-E'} + \frac{E-E_r}{V_E^*}\delta(E-E')\right). \tag{4.0.32}$$

This completes the solution of the system of equations (4.0.9) and (4.0.11). Let us now consider the structure of the newly constructed continuum wave function $\Psi_E(x)$ from Eq. (4.0.7). Ψ_E is a superposition of unperturbed continuum waves $\Psi_{E'}$ with maximum height at $E = E'$ as well as of the bound state ϕ_0 and is characterized by a wave function which is localized at a finite distance, e.g. Bohr's radius, and decays rapidly in the asymptotic region. The strength of this localized contribution to $\Psi_E(x)$ is written as,

$$|\langle\phi_0|\Psi_E\rangle|^2 = |a(E)|^2 = \frac{\Gamma_E/2\pi}{(E-E_r)^2+\Gamma_E^2/4} \tag{4.0.33}$$

has a maximum at the resonance energy $E = E_r$. Rigorously this is an implicit equation, because E_r itself depends (weakly) on E through the principal value integral $F(E)$ and $F(E)$ describes the additional level shift due to the coupling to the continuum. If one moves away from E_r in energy the admixture Eq. (4.0.33) falls off on a scale determined by the resonance widthΓ_E. Equation Eq. (4.0.33) has the shape of a Breit-Wigner curve characteristic of resonances. The enhancement of the wave function Ψ_E near the resonance is displayed schematically in Fig.4.1 for the case of an attractive potential well.

The asymptotic behavior of the wave function ψ_E for $r \to \infty$ examined using Eqs. (4.0.7), (4.0.30), and (4.0.32). For simplicity, we restrict ourselves to the non-relativistic case (the Schrodinger equation) with a rapidly decreasing central potential. The unperturbed continuum wave ψ_E then behaves like

$$\psi_E(r) \to N_E sin(pr + \delta_E), \tag{4.0.34}$$

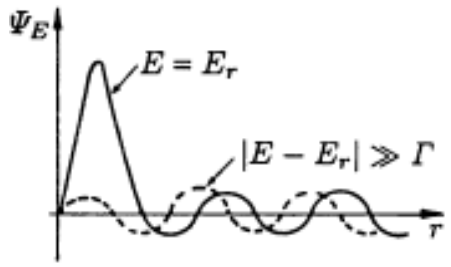


Figure 4.1: The wave function $\psi_E(r)$ in the vicinity of the resonance and far away from it

with momentum $p = \sqrt{2mE}$ and a normalization constant N_E. The information about the effective scattering potential is contained in the phase shift δE. The new continuum wave function Ψ_E depends on r like

$$\begin{aligned}\Psi_E(r) &= a(E)\phi_0 + \int dE' h'_E(E)\psi_{E'}(r) \\ &\to a(E)\int dE'\left(p\frac{V_{E'}}{E-E'} + \frac{E-E_r}{V_E^*}\delta(E-E')\right)N_{E'}sin(p'r+\delta_{E'}),\end{aligned} \tag{4.0.35}$$

where we have used the fact that $\phi_0(r)$ asymptotically approaches zero. By use of the identity

$$p\frac{1}{x} = \frac{1}{2}\left(\frac{1}{x+i\epsilon} + \frac{1}{x-i\epsilon}\right), \tag{4.0.36}$$

then, the principal value integral in Eq. (4.0.35) give as

$$\begin{aligned}&\int dE' p\frac{V_{E'}}{E-E'}N_{E'}sin(p'r+\delta_{E'}) \\ = \quad &\frac{i}{4}\int dE' V_{E'}N_{E'}\left(\frac{1}{E'-E-i\epsilon} + \frac{1}{E'-E+i\epsilon}\right) \\ &\times\left(e^{i(p'r+\delta_{E'})} - e^{-i(p'r+\delta_{E'})}\right).\end{aligned} \tag{4.0.37}$$

This integral has simple poles at $E' = E \pm i\epsilon$. It can easily be solved by use of the theorem of residues if the limits of integration are extended to infinity, see Fig.4.2. (This is an approximation since in reality the continuous spectrum is bounded on one side, e.g. $0 < E' < \infty$ in the non-relativistic case or $mc^2 < |E'| < \infty$ for the Dirac equation.) The

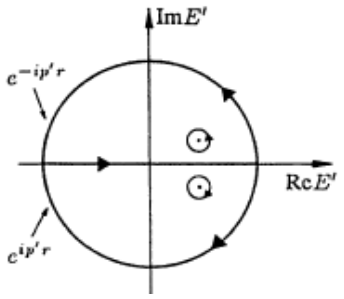


Figure 4.2: Integration contours in Eq. (4.0.37)

integration contour then can be closed by a semicircle at infinity. If the principal value of the square root in the complex plane is chosen for $p' = \sqrt{2mE'}$,

$$sin(Im\{p'\}) = sin(Im\{E'\}), \tag{4.0.38}$$

then the contour has to be closed in the upper (lower) half plane for the case $e^{ip'r}(e^{-ip'r})$. Two of the four integrals in Eq. (4.0.37) vanish provided that $V_{E'}N_{E'}$ is holomorphic; the remaining two integrals yield

$$\pm\frac{i}{4}\int_{-\infty}^{\infty} dE' V_{E'} N_{E'} \frac{e^{i\pm(p'r+\delta_{E'})}}{E' - E \mp i\epsilon} = -\frac{\pi}{2} V_E N_E e^{\pm i(pr+\delta_E)}. \tag{4.0.39}$$

This leads to

$$\int dE' p \frac{V_{E'}}{E - E'} N_{E'} sin(p'r + \delta_{E'}) = -\pi V_E N_E cos(pr + \delta_E). \tag{4.0.40}$$

Hence Eq. (4.0.35) combined with the Eq. (4.0.30) gives

$$\begin{aligned}
&\Psi_E(r) \to a(E)\Big[-\pi V_E N_E cos(pr + \delta_E) + \big(\frac{(E - E_r)}{V_E^*}\big) N_E sin(pr + \delta_E)\Big] \\
&= \frac{N_E}{\sqrt{(E - E_r)^2 + \Gamma_E^2/4}}\Big[-(\frac{\Gamma_E}{2}) cos(pr + \delta_E) + (E - E_r) sin(pr + \delta_E)\Big] \\
&= N_E sin(pr + \delta_E + \Delta_E),
\end{aligned} \tag{4.0.41}$$

with the phase shift

$$\Delta_E = -arctan\frac{\Gamma_E/2}{E - E_r}. \tag{4.0.42}$$

The modified continuum wave $\Psi_E(r)$ thus displays exactly the same asymptotic behavior as $\psi_E(r)$ but it is shifted by an angle Δ_E. As Fig.4.3 shows, the phase shift is nearly constant for $|E - E_r| \gg \Gamma_E \sim \Gamma_{E_r}$ and has no effect in Eq. (4.0.41). In the vicinity of E_r, however, it "jumps"very rapidly by an angle of π. This behavior is well known from the quantum-mechanical theory of resonant scattering.

Finally, let us express the expansion coefficients $a(E)$, $h_{E'}(E)$ in terms of the phase shift. Equation (4.0.31) yields

$$\begin{aligned} a(E) &= \frac{1}{\pi V_E} \frac{\Gamma_E/2}{\sqrt{(E-E_r)^2 + \Gamma_E^2/4}} \\ &= \frac{1}{\pi V_E} \sqrt{\frac{tan^2\Delta_E}{1+tan^2\Delta_E}} = \frac{sin\Delta_E}{\pi V_E} \end{aligned} \tag{4.0.43}$$

and Eq. (4.0.32) becomes

$$\begin{aligned} h_{E'}(E) &= \frac{sin\Delta_E}{\pi V_E} P\frac{V_{E'}}{E-E'} + sin\Delta_E \frac{E-E_r}{\pi |V_E|^2} \delta(E-E') \\ &= \frac{sin\Delta_E}{\pi V_E} P\frac{V_{E'}}{E-E'} - cos\Delta_E \delta(E-E'). \end{aligned} \tag{4.0.44}$$

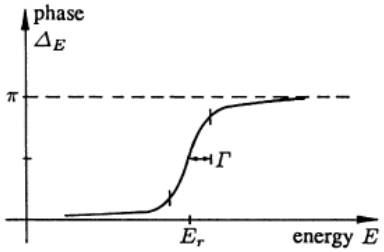


Figure 4.3: The additional phase shift Δ_E in the vicinity of the resonance

4.1 The product of two principal-value poles

We want to prove the identity

$$\begin{aligned} P\frac{1}{E-E''} P\frac{1}{E'-E''} = \quad & P\frac{1}{E-E'}\left(P\frac{1}{E'-E''} - P\frac{1}{E-E''}\right) \\ & +\pi^2 \delta(E-E'')\delta(E'-E''), \end{aligned} \tag{4.1.1}$$

which displays the behavior of the product of two principal-value singularities as a function of $E' - E$. In-order to proof we use the identity

$$\frac{1}{x \pm i\epsilon} = P\frac{1}{x} \mp i\pi\delta(x), \tag{4.1.2}$$

which holds in the limit $\epsilon \to +0$. Now the left hand side can be written as

$$\begin{aligned}
&\left(\frac{1}{E - E'' + i\epsilon} + i\pi\delta(E - E'')\right)\left(\frac{1}{E' - E'' - i\epsilon'} - i\pi\delta(E' - E'')\right) \\
&= \frac{1}{(E - E'' + i\epsilon)(E' - E'' - i\epsilon')} + i\pi\frac{\delta(E' - E'')}{(E' - E'' - i\epsilon')} \\
&-i\pi\frac{\delta(E' - E'')}{(E - E'' + i\epsilon)} + \pi^2\delta(E - E'')\delta(E' - E''). \qquad (4.1.3)
\end{aligned}$$

The relation

$$\begin{aligned}
&P\frac{1}{E - E'}\left(P\frac{1}{E' - E''} - P\frac{1}{E - E''}\right) \\
= \quad &\left(\frac{1}{E - E' + i\epsilon} + i\pi\delta(E = E')\right) \\
&\times\left(\frac{1}{E' - E'' - i\epsilon'} - i\pi\delta(E' - E'') - \frac{1}{E - E'' + i\epsilon''} - i\pi\delta(E - E'')\right) \qquad (4.1.4)
\end{aligned}$$

holds for the first term on the right-hand side of the conjecture. The delta function in the first factor can be omitted, because the second factor vanishes for $E = E'$,

$$\begin{aligned}
\frac{1}{E - E' + i\epsilon} \quad &\left(\frac{1}{E' - E'' - i\epsilon'} - \frac{1}{E - E'' + i\epsilon''}\right) \\
&+i\pi\frac{\delta(E - E'')}{E' - E'' - i\epsilon} - i\pi\frac{\delta(E' - E'')}{(E - E'' + i\epsilon)} \\
= \quad &\frac{(E - E'' + i\epsilon'') - (E' - E'' - i\epsilon')}{(E - E' + i\epsilon)(E' - E'' - i\epsilon')(E - E'' + i\epsilon'')} \\
&+i\pi\frac{\delta(E - E'')}{(E' - E'' - i\epsilon)} - i\pi\frac{\delta(E' - E'')}{(E - E'' + i\epsilon)}. \qquad (4.1.5)
\end{aligned}$$

Keeping in mind that ϵ, ϵ', ϵ'' are infinitesimal quantities whose value does not matter, the first factor can be canceled in the denominator. Then we obtain

$$\begin{aligned}
\frac{1}{E - E' + i\epsilon} \quad &\left(\frac{1}{E' - E'' - i\epsilon'} - \frac{1}{E - E'' + i\epsilon''}\right) \\
&+i\pi\frac{\delta(E - E'')}{E' - E'' - i\epsilon} - i\pi\frac{\delta(E' - E'')}{(E - E'' + i\epsilon)} \\
&= i\pi\frac{\delta(E - E'')}{(E' - E'' - i\epsilon)} - i\pi\frac{\delta(E' - E'')}{(E - E'' + i\epsilon)}. \qquad (4.1.6)
\end{aligned}$$

Now Comparison of Eqs. (4.1.6) and (4.1.3) proves the conjecture Eq. (4.1.1).

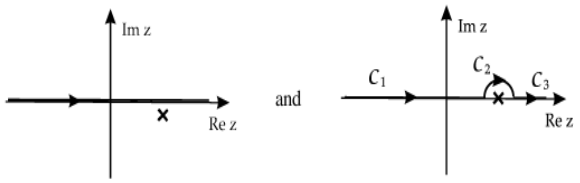
It is perhaps helpful to remember the proof of Eq. (4.1.2), i.e.

$$\frac{1}{z-z_0+i\epsilon} = P\frac{1}{z-z_0} - i\pi\delta(z-z_0). \tag{4.1.7}$$

It has to be shown that in the limit as $\epsilon \to 0$

$$I = \int_{-\infty}^{\infty} dz \frac{f(z)}{z-z_0+i\epsilon} = \left[\int_{-\infty}^{z_0-\epsilon} dz + \int_{z_0+\epsilon}^{\infty} dz\right]\frac{f(z)}{z-z_0} - i\pi f(z_0), \tag{4.1.8}$$

holds. Now, for $\epsilon \to 0$ the integration paths, are equivalent. Therefore



$$I = \int_c dz \frac{f(z)}{z-z_0+i\epsilon} = \left[\int_{-\infty}^{z_0-\epsilon} dz + \int_{c_2} dz + \int_{z_0+\epsilon}^{\infty} dz\right]\frac{f(z)}{z-z_0}. \tag{4.1.9}$$

The sum of the first and third term in the brackets defines the principal-value integral. Assuming that the test function $f(z)$ is regular at $z = z_0$ the remaining integral over the semicircle C_2 yields

$$\begin{aligned}\int_{c_2} dz \frac{f(z)}{z-z_0+i\epsilon} &\simeq f(z_0)\int_{c_2} dz \frac{1}{z-z_0+i\epsilon} = \frac{1}{2}f(z_0)\oint dz \frac{1}{z-z_0+i\epsilon} \\ &= \frac{1}{2}f(z_0)(-2\pi i).\end{aligned} \tag{4.1.10}$$

4.2 Time-dependent decay of the vacuum

We now want to calculate the final hole probability in the bound state and the spectrum of the emitted positrons depending on the diving duration using Fano's formalism. The potential strength is increased suddenly at the time $t = 0$ so that the state which previously was bound slightly sub-critically becomes a resonance in the lower continuum.

The sub-critical system is restored at $t = T$ by reducing the potential strength. The Hamiltonian is now a function of time is given by,

$$H(t) = \begin{cases} H_0, & for\ t\ <\ 0 \\ H_0 + V', & for\ 0 \leq\ t \leq\ T. \\ H_0, & for\ t\ >\ T \end{cases} \tag{4.2.1}$$

A time-dependent wave function $\Psi(t)$ has to be constructed in such a way that it describes a bound hole state ϕ_0 for $t < 0$. A piecewise ansatz can be made for $\Psi(t)$ in the three regions as

$$\Psi(t) = \begin{cases} \phi_0 e^{-iE_0 t}, & for\ t\ <\ 0 \\ \int dE \tilde{c}(E) \Psi_E e^{-iEt}, & for\ 0 \leq\ t \leq\ T. \\ c_0 \phi_0 e^{-iE_0(t-T)} + \int dE c(E) \psi_E e^{-iE(t-T)}, & for\ t\ >\ T \end{cases} \tag{4.2.2}$$

The expansion coefficients $\tilde{c}(E)$ or c_0 and $c(E)$ are independent of time since by assumption the wave functions Ψ_E or ψ_E and ϕ_0 are eigenstates of the Hamiltonians H or H_0 respectively. Hence they develop freely with a time dependence $\exp(-iEt)$. $\Psi(t)$ is required to be continuous at $t = 0$ and $t = T$. This means that

$$\phi_0 = \int dE \tilde{c}(E) \Psi_E, \tag{4.2.3}$$

and

$$\int dE \tilde{c}(E) \Psi_E e^{-iEt} = c_0 \phi_0 + \int dE c(E) \Psi_E. \tag{4.2.4}$$

By projection onto $\langle \Psi_E |$ or $\langle \phi_0 |$ and $\langle \psi_E |$, equations determining the coefficients $\tilde{c}(E)$ and $c(E)$ are obtained using Eqs. (4.0.3) and (4.0.8).

$$\tilde{c}(E) = a^*(E). \tag{4.2.5}$$

$$c_0 = \int dE \tilde{c}(E) a(E) e^{-iEt} = \int dE a^*(E) a(E) e^{-iET}. \tag{4.2.6}$$

$$c(E) = \int dE' \tilde{c}(E') h_E(E') e^{-iE'T} = \int dE a^*(E') h_E(E') e^{-iE'T}. \tag{4.2.7}$$

The integration interval extends from $E = -\infty$ to $E = -m_0c^2$. In order to be able to proceed with an analytical calculation we make an approximation Eq. (4.1.10) and replace the upper limit by $E = +\infty$. The integrals can be solved by residue integration with the assumption that the matrix element $V_E = \langle \Psi_E | V' | \Phi \rangle$ is an analytic function of energy.

Using Eq. (4.0.33) the discrete expansion coefficient follows as

$$c_0 = \int_{-\infty}^{+\infty} dE \frac{\Gamma_E/2\pi}{(E - E_r)^2 + \Gamma_E^2/4} e^{-iET} = e^{-iE_rT} e^{-\Gamma_0 T/2}, \tag{4.2.8}$$

where $\Gamma_0 = \Gamma_E = E_r$ is the width Γ_E at the resonance energy E_r . Here the integration path has been closed in the lower half-plane. The relevant quantity is the squared absolute value of c_0 ,

$$P_0(T) = |c_0|^2 = e^{-\Gamma_0 T}. \tag{4.2.9}$$

This is the probability of finding a hole in state ϕ_0 after a time T thus decreases exponentially as determined by the decay width $\Gamma_0 = \Gamma_{E_r}$. In order to see how the positron probability correspondingly builds up with time, the integral (see Eqs. (4.2.7), (4.0.14) and (4.0.21) for $h_E(E)$)

$$c(E) \simeq \int_{-\infty}^{+\infty} dE' \frac{|V_{E'}|^2}{(E' - E_r)^2 + \Gamma_{E'}^2/4} \left(P \frac{V_E}{E' - E} + \frac{E - E_r}{V_E^*} \delta(E - E') \right) e^{-iE'T}. \tag{4.2.10}$$

Now we reformulate the principal-value term

$$P \frac{V_E}{E' - E} = \frac{V_E}{E' - E - i\epsilon} - i\pi V_E \delta(E - E'), \tag{4.2.11}$$

which is useful because a pole in the upper half-plane does not contribute. Eq. (4.2.10) give as

$$\begin{aligned} c(E) \simeq \quad & \int_{-\infty}^{+\infty} dE' \frac{|V_{E'}|^2}{(E' - E_r)^2 + \Gamma_{E'}^2/4} \frac{V_E}{E' - E - i\epsilon} e^{-iE'T} \\ & + \frac{V_E}{(E - E_r)^2 + \Gamma_E^2/4} (E - E_r - i\pi |V_E|^2) e^{-iET}. \end{aligned} \tag{4.2.12}$$

Only the pole at the point $E' = E_r - i\Gamma_0/2$ contributes in the residue integration. The second term in Eq. (4.2.12) can be simplified as, since $|V_E|^2 = \Gamma_0/2\pi$

$$c(E) \simeq \frac{V_E}{E - E_r + i\Gamma_E/2} e^{-iET} - \frac{V_{E_r}}{E - E_r + i\Gamma_0/2} e^{-iE_rT} e^{-i\Gamma_0 T/2}. \tag{4.2.13}$$

The energy spectrum of the produced positrons is given by the absolute squared of the expansion coefficient $c(E)$. With the assumption that Γ_E depends only weakly on E and can be replaced by Γ_0 we obtain

$$\frac{dP}{dE} = |c(E)|^2 = \frac{\Gamma_0/2\pi}{(E - E_r + \Gamma_0^2/4)} |1 - e^{i(E-E_r)T} e^{-\Gamma_0 T/2}|^2. \tag{4.2.14}$$

It can be checked that the norm of the wave function $\Psi(t)$ is conserved in spite of the diverse approximations, i.e.

$$\int_{-\infty}^{+\infty} dE \frac{dP}{dE} = 1 - e^{-\Gamma_0 T} = 1 - P_0(T). \tag{4.2.15}$$

To see this we evaluate the integral

$$\begin{aligned} \int_{-\infty}^{+\infty} \frac{dP}{dE} &= \frac{\Gamma_0}{2\pi} \int_{-\infty}^{+\infty} dE \frac{1 - 2cos[(E - E_r)T] e^{-\Gamma_0 T/2} + e^{-\Gamma_0 T}}{(E - E_r)^2 + \Gamma_0^2/4} \\ &= \frac{1}{\pi} \int_{-\infty}^{+\infty} dx \frac{1 - 2cos(\frac{\Gamma_0 T}{2} x) e^{-\Gamma_0 T/2} + e^{-\Gamma_0 T}}{1 + x^2}. \end{aligned} \tag{4.2.16}$$

where the variable transformation $x = 2(E - E_r)/\Gamma_0$ was performed. Employing the standard integral

$$\int_{-\infty}^{+\infty} dx \frac{cos(ax)}{1 + x^2} = \pi e^{-|a|}, \tag{4.2.17}$$

we find

$$\begin{aligned} \int_{-\infty}^{+\infty} dE \frac{dP}{dE} &= \frac{1}{\pi}(1 - 2e_{-\Gamma_0 T/2}) e_{-\Gamma_0 T/2} + e^{-\Gamma_0 T} \\ & 1 - e^{\Gamma_0 T} = 1 - P_0(T). \end{aligned} \tag{4.2.18}$$

This assures the conservation of probability:

$$P_0(T) + \int_{-\infty}^{+\infty} dE \frac{dP}{dE} = 1 \quad or \quad |c_0|^2 + \int_{-\infty}^{+\infty} dE |c(E)|^2 = 1. \tag{4.2.19}$$

for all times T.

Now let us discus two limiting cases of the spectrum Eq. (4.2.14), see Fig. 4.4.

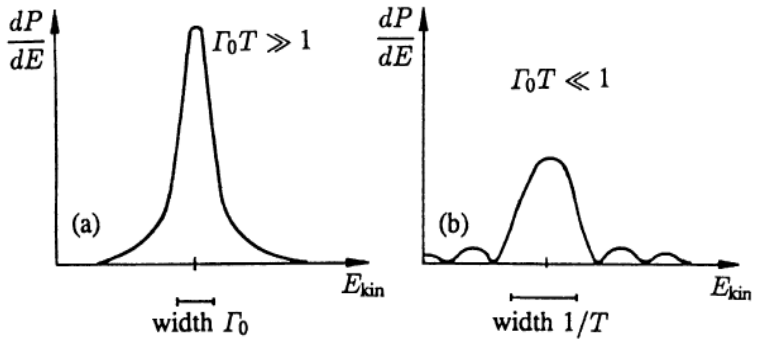


Figure 4.4: The spectra of emitted positrons in the limits of a large (a) and small (b) time of super criticality T

a) $\Gamma_0 T \gg 1$: If the diving time is large compared to the natural decay time $1/\Gamma_0$, a Breit-Wigner spectrum with line width Γ_0 results:

$$\frac{dP}{dE} = \frac{\Gamma_0/2\pi}{(E-E_r)^2 + \Gamma_0^2/4}. \tag{4.2.20}$$

b) $\Gamma_0 T \ll 1$: If the potential is supercritical only during a short time interval T, then

$$\frac{dP}{dE} = \frac{\Gamma_0}{2\pi}\frac{|1-e^{i(E-E_r)T}|^2}{(E-E_r)^2} = \frac{\Gamma_0 T^2}{2\pi}\left[\frac{sin(E-E_r)T/2}{(E-E_r)T/2}\right]^2. \tag{4.2.21}$$

This is an oscillating function with maximum at $E = E_r$ having a width decreasing with the inverse of T. The peak height increases quadratically and it consistent linearly in T until saturation is reached at $T > 1/\Gamma_0$.

Chapter 5

Conclusion

In this thesis we have obtained the system of two coupled ordinary differential equation of the radial wave functions u_1 and u_2 for the Ddirac particles. Then using this we have derived Sommerfeld expression for energy eigenvalues for electrons bound to nuclei. Applying the wave function at the diving point, we have determined the second order differential equation of wave function u_1, and the modified Bessel's differential equation of wave function u_1.

Employing the Sommerfeld fine-structure formula, we have calculated the binding energies for $1s_{1/2}$ electrons of nuclear charge Z, and we have obtained the classification of bound states of the electron according to the Dirac equation for nuclear charge $Z = 1$ (hydrogen atom) by calculating the quantum numbers k, j, n', and l for the given value of the principal quantum number n. We have found that the energy levels descend progressively with increasing nuclear charge Z. The energy of the lowest state ($1s$, $k = 1$) becomes negative when nuclear charge $Z > 150$ and $1s$ level finally reaches the value $E_{1s} = -m_0c^2$ at a critical charge $Z_{cr}^{1s} \backsimeq 173$, and the Sommerfeld energies of the states with $k = -1(ns_{1/2})$ and $k = +1(np_{1/2})$ break off with a vertical tangent at $Z\alpha = 1$ and with the finite nuclear radius taken into account all levels reach the edge of the lower continuum $E = -m_0c^2$ at a corresponding critical charge Z_{cr}.

Moreover, using perturbation potential V' we have develop the Fano's formalism for the description of resonances. Then we have calculated the final hole probability in the bound

state and the spectrum of the emitted positrons depending on the diving duration. We have found that the modified continuum wave $\Psi_E(r)$ displays exactly the same asymptotic behavior as $\psi_E(r)$ but it is shifted by an angle

$$\Delta_E = -arctan\frac{\Gamma_E/2}{E - E_r}.$$

The phase shift is nearly constant for $|E - E_r| \gg \Gamma_E \sim \Gamma_{E_r}$ and has no effect in the modified continuum wave $\Psi_E(r)$. Furthermore, we found that the probability of finding a hole in a state ϕ_0 after time T is

$$P_0(T) = |c_0|^2 = e^{-\Gamma_0 T},$$

which decreases exponentially. And the energy spectrum of the produced positrons is

$$\frac{dP}{dE} = |c(E)|^2 = \frac{\Gamma_0/2\pi}{(E - E_r + \Gamma_0^2/4)}|1 - e^{i(E-E_r)T}e^{-\Gamma_0 T/2}|^2.$$

From this, an oscillating function with maximum at $E = E_r$ having a width decreasing with the inverse of T, the peak height increases quadratically and it consistent linearly in T until saturation is reached at $T > 1/\Gamma_0$.

References

[1] A.W. Stetz, Introduction to Quantum Field Theory, (Nov. 21, 2007).

[2] B. Muller, J. Rafelski, W. Greiner: Z. Physik 257, 62 and 183 (1972).

[3] U. Fano: Phys. Rev. 124, 1866 (1961).

[4] L. Fonda et al.: Rep. Progr. Phys. Rev. 41, 587 (1978).

[5] M.E. Rose, Relativistic Electron Theoiy, (Wiley, New York, London).

[6] J.M. Jauch, F. Rohrlich: The Theory of Photons and Electrons, (Springer-Verlag, 2006).

[7] P. Schmelcher, W. Schweizer: Atoms and molecules in Strong External Fields, (Proc. 172 and Bad Honnef Seminar, Springer, 1997).

[8] P. Gartner, U. Heinz, B. Muller, W. Greiner, Z. Physik. A 300, 143 (1981).

[9] Claude Cohen-Tannoudji, Photons and Atoms to Quantum Electrodynamics, (Wiley Professional, 1997).

[10] W. Greiner, B. Muller: Quantum Mechanics - Symmetries, 2nd ed.(Springer, Berlin, Heidelberg, 1994).

[11] P.H. Mokler, Quantum Electrodynamics Contribution to Atomic Structure at Strong Central Fields, Radiation Physics and Chemistry, 75, 1730 (2006).

[12] G. Soff et al Quantum Electrodynamics of Strong Fields, Status and Perspectives, Advances on Quantum Chemistry, 30, 125 (1998).
New York, 1965).

[13] G. Soff et al Phys. Rev. lett. 48, 1465 (1982).

[14] Franz Gross, Relativistic Quantum mechanics and Field Theory, (Wiley Science Paperback Series, 1999).

[15] David Atkinson, Porter Wear Johnson, Quantum Field Theory: A self Contained Course, Volume 2 (2003).

[16] Peter W. Milonni, The Quantum Vacuum: An Introduction to Quantum Electrodynamics, (Academic Press, 1993).

[17] M. Abramowitz, I.A. Stegun: Handbook of Mathematical Functions (Dover,

[18] Donald A.McQuarric, Peter A. Rock, General Chemistry, 3rd ed.(New York, 1991).

Declaration

This thesis is my original work, has not been presented for a degree in any other University and that all the sources of material used for the thesis have been dully acknowledged.

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