((**Sakurai 8-7**))

This problem is taken from Quantum Mechanics II: A Second Course in Quantum Theory, 2nd edition, by Rubin H. Landau (1996) p.212. A spin-less electron is bound by the Coulomb potential

$$V(r) = -\frac{Ze^2}{r},$$

in a stationary state of total energy ($E \le mc^2$). You can incorporate this interaction into the Klein-Gordon equation by using the covariant derivative with $V = e\Phi$ and $\boldsymbol{A} = 0$.

(a)Assume that the radial and angular parts of the equation separate and that the wave function can be written as

$$e^{-\frac{iEt}{\hbar}}[\frac{u_l(r)}{r}]Y_{lm}(\theta,\phi)$$

Show that the radial equation becomes

$$\frac{d^2u_l(\rho)}{d\rho^2} + [\frac{2EZ\alpha}{\gamma\rho} - \frac{1}{4} - \frac{l(l+1)-(Z\alpha)^2}{\rho^2}]u_l(\rho) = 0$$

where $\alpha = e^2$, $\gamma^2 = 4(m^2 - E^2)$, and $\rho = \gamma r$.

(b) Assume that this equation has a solution of the usual form of a power series times the $\rho \to \infty$ and $\rho \to 0$ solutions, that is,

$$u_l(\rho) = \rho^k(1 + c_1\rho + c_2\rho^2 + ...)e^{-\rho/2}$$

and show that

$$k = k_\pm = \frac{1}{2} \pm \sqrt{(l+\frac{1}{2})^2 - (Z\alpha)^2}$$

and that only for $k_+$ is the expectation value of the kinetic energy finite and that this solution has a nonrelativistic limit that agrees with the solution found for the Schrödinger equation.

(c) Determine the recurrence relation among the $c_i's$ for this to be a solution of the Klein-Gordon equation, and show that unless the power series terminates, the wave function will have an incorrect asymptotic form.

(d) In the case where the series terminates, show that the energy eigenvalue for the $k_+$ solution is

$$E = \frac{mc^2}{\sqrt{1 + \frac{(Z\alpha)^2}{[n - l - \frac{1}{2} + \sqrt{(l + \frac{1}{2})^2 - (Z\alpha)^2}]^2}}}$$

where $n$ is the principal quantum number.

(e) Expand $E$ in powers of $(Z\alpha)^2$ and show that the first-order term yields the Bohr formula. Connect the higher-order terms with relativistic corrections, and discuss the degree to which the degeneracy in $l$ is removed.

((**Notation**))

$$p^\mu = i\hbar\partial^\mu = i\hbar\frac{\partial}{\partial x_\mu} = (\frac{\varepsilon}{c}, \boldsymbol{p}), \qquad p_\mu = i\hbar\partial_\mu = i\hbar\frac{\partial}{\partial x^\mu} = (\frac{\varepsilon}{c}, -\boldsymbol{p})$$

$$\varepsilon = i\hbar\frac{\partial}{\partial t}, \qquad \boldsymbol{p} = -i\hbar\nabla$$

$$p^\mu p_\mu = p^0 p_0 - \boldsymbol{p}^2 = \frac{\varepsilon^2}{c^2} - \boldsymbol{p}^2 = m^2c^2$$

where $A^0$ is a scalar potential and $\boldsymbol{A}$ is a vector potential,

$$A^\mu = (A^0, \boldsymbol{A}), \qquad A_\mu = (A^0, -\boldsymbol{A})$$

((**Solution**))
We start with the Klein-Gordon equation

$$\varepsilon^2 = m^2c^4 + c^2\boldsymbol{p}^2$$

In the presence of the field,

$$p^\mu \to p^\mu - \frac{e}{c}A^\mu, \qquad p_\mu \to p_\mu - \frac{e}{c}A_\mu$$

or

$$\partial^\mu \to \partial^\mu + \frac{ie}{c\hbar}A^\mu, \qquad \partial_\mu \to \partial_\mu + \frac{ie}{c\hbar}A_\mu$$

where $e$ is the charge of the particle ($e$<0 for electron)

$$\frac{\varepsilon}{c} \to \frac{1}{c}i\hbar\frac{\partial}{\partial t} - \frac{e}{c}\Phi_0, \qquad \text{or} \qquad \varepsilon \to i\hbar\frac{\partial}{\partial t} - e\Phi_0$$

(a)

Klein-Gordon equation

$$[(\frac{i\hbar}{c}\frac{\partial}{\partial t} - e\Phi_0)^2 - (\frac{\hbar}{i})^2\nabla^2 - m^2c^2]\psi = 0$$

or

$$[\frac{i\hbar}{c}\frac{\partial}{\partial t} - V(r)^2]\psi(\boldsymbol{r},t) + (\hbar^2\nabla^2 - m^2c^2)\psi(\boldsymbol{r},t) = 0$$

with

$$e\Phi_0 = V(r) = -\frac{Ze^2}{r}$$

Suppose that $\psi(r,t) = e^{-\frac{iEt}{\hbar}}\psi(r)$

$$\{[\frac{E}{c} - V(r)]^2 + \hbar^2(\nabla^2 - \frac{m^2c^2}{\hbar^2})\psi(\boldsymbol{r},t) = 0$$

or

$$[\frac{1}{\hbar^2}(\frac{E}{c}+\frac{Ze^2}{r})^2+\nabla^2-\frac{m^2c^2}{\hbar^2}]\psi(\mathbf{r},t)=0$$

Noting that

$$\nabla^2=\frac{1}{r}\frac{\partial^2}{\partial r^2}r-\frac{l(l+1)}{r^2}$$

we have the second-order differential equation

$$[\frac{1}{\hbar^2}(\frac{E}{c}+\frac{Ze^2}{r})^2+\frac{1}{r}\frac{\partial^2}{\partial r^2}r-\frac{l(l+1)}{r^2}-\frac{m^2c^2}{\hbar^2}]R_l(r)=0\,.$$

We put $u_l(r)=rR_l(r)$

$$[\frac{1}{\hbar^2}(\frac{E}{c}+\frac{Ze^2}{r})^2-\frac{l(l+1)}{r^2}-\frac{m^2c^2}{\hbar^2}]u_l(r)+\frac{1}{r}\frac{\partial^2}{\partial r^2}u_l(r)=0$$

Using the fine structure constant $\alpha$

$$[(\frac{E}{c\hbar}+\frac{Z\alpha}{r})^2-\frac{l(l+1)}{r^2}-\frac{m^2c^2}{\hbar^2}]u_l(r)+\frac{\partial^2}{\partial r^2}u_l(r)=0$$

where

$$\alpha=\frac{e^2}{c\hbar}.$$

Finally, with

$$\gamma^2=4(\frac{m^2c^4-E^2}{c^2\hbar^2}) \qquad \text{and} \qquad \rho=\gamma r$$

this becomes

$$\frac{d^2u}{d\rho^2}+[\frac{2EZ\alpha}{c\hbar\gamma\rho}-\frac{1}{4}-\frac{l(l+1)-(Z\alpha)^2}{\rho^2}]u=0$$

(b)
For $\rho\to\infty$, this equation becomes

$$\frac{d^2u}{d\rho^2}-\frac{1}{4}u=0$$

The solution is

$$u=e^{\pm\frac{\rho}{2}}$$

So we can write the form of the solution for *u* as

$$u=e^{-\frac{\rho}{2}}w(\rho)$$

Thus we have

$$\frac{d^2w}{d\rho^2}-\frac{dw}{d\rho}+[\frac{2EZ\alpha}{c\hbar\gamma\rho}-\frac{l(l+1)-(Z\alpha)^2}{\rho^2}]w=0$$

((**Series expansion**)) We solve this differential equation using the series expansion. We use the Mathematica.

(c) We assume that

$$w(\rho)=\rho^k[C(0)+C(1)\rho+C(2)\rho^2+......]$$

where $C(0)\neq 0$. Using the Mathematica, we get

$$c\gamma\hbar(-k+k^2-l-l^2+Z^2\alpha^2)C(0)=0\,, \qquad (1)$$

$$2EZ\alpha C(0)+c\gamma\hbar\{-kC(0)+[k(k+1)-l(l+1)+Z^2\alpha^2]C(1)\}=0$$

$$2EZ\alpha C(1)+c\gamma\hbar\{-(k+1)C(1)+[(k+1)(k+2)-l(l+1)+Z^2\alpha^2]C(2)\}=0$$

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In general we have the relation

$$C(n+1) = -\frac{1}{c\gamma\hbar}\ \frac{[2EZ\alpha - c\gamma\hbar(k+n)]}{k(k+1) - l(l+1) + n + 2kn + n^2 + Z^2\alpha^2} C(n).$$

The value of k can be determined from Eq.(1) as

$$k_{\pm} = \frac{1}{2} \pm \sqrt{(l+\frac{1}{2})^2 - Z^2\alpha^2}$$

We choose $k = k_{+}$

We find the condition that $C(n_r) \neq 0$, but $C(n_r + 1) = 0$. If it is so, $C(n_r + 2) = C(n_r + 3) = .... = 0$. So the series terminates up to $C(n)$. The condition for this is

$$2EZ\alpha - c\gamma\hbar(k + n_r) = 0$$

with

$$\gamma = \frac{2}{c\hbar}\sqrt{m^2c^4 - E^2}\ , \quad k_{+} = \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - Z^2\alpha^2}\ ]$$

Here we introduce the principal quantum number $n = n_r + l + 1$. Then we have

$$E = -\frac{mc^2[n - (l+\frac{1}{2}) + \sqrt{(l+\frac{1}{2})^2 - Z^2\alpha^2})}{\sqrt{[n - (l+\frac{1}{2}) + \sqrt{(l+\frac{1}{2})^2 - Z^2\alpha^2}\ ]^2 + Z^2\alpha^2}}]$$

$$= \frac{mc^2}{\sqrt{1 + \frac{Z^2\alpha^2}{[n - (l+\frac{1}{2}) + \sqrt{(l+\frac{1}{2})^2 - Z^2\alpha^2}\ ]^2}}}$$

The energy E can be expanded in a series of $\alpha^2$

$$E = mc^2 - \frac{mc^2}{2n^2}(Z\alpha)^2 + \frac{mc^2}{8n^4}\frac{(6l+3-8n)}{(2l+1)}(Z\alpha)^4 + ...$$

This result is compared with the exact solution from the Dirac theory.

$$E = \frac{mc^2}{\sqrt{1 + \frac{Z^2\alpha^2}{[n-(j+\frac{1}{2})+\sqrt{(j+\frac{1}{2})^2 - Z^2\alpha^2}]^2}}}$$

In the Dirac theory, the energy level depends only on $n$ and $j$, but not $l$

It is surprising that the energy level derived from the Klein-Gordon equation is the same as that derived from the Dirac theory when $j$ is replaced by $l$ in the Dirac theory.

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((**Solution**)) Mathematica

```
Clear["Global`*"];

eq1 = u''[ρ] + (2 E1 Z α/(c ħ γ ρ) - 1/4 - (L1 (L1 + 1) - (Z α)^2)/ρ^2) u[ρ];

rule1 = {u → (Exp[-#/2] w[#] &)};

eq2 = eq1 /. rule1 // Simplify

(e^(-ρ/2) ((2 E1 Z α ρ - c (L1 + L1^2 - Z^2 α^2) γ ħ) w[ρ] + c γ ρ^2 ħ (-w'[ρ] + w''[ρ])))/(c γ ρ^2 ħ)

eq3 = ((2 E1 Z α ρ - c (L1 + L1^2 - Z^2 α^2) γ ħ) w[ρ] + c γ ρ^2 ħ (-w'[ρ] + w''[ρ]));

rule2 = {w → (Sum[C[s] #^(k+s), {s, 0, 10}] &)};

eq4 = eq3/ρ^k /. rule2 // Expand;
```

```
list1 = Table[{s, Coefficient[eq4, ρ, s]}, {s, 0, 5}] // FullSimplify; list1 // TableForm
```

| | |
|---|---|
| 0 | $c\left((-1+k)\,k - L1\,(1+L1) + Z^2\alpha^2\right)\gamma\hbar\, C[0]$ |
| 1 | $2\,E1\,Z\,\alpha\, C[0] + c\,\gamma\,\hbar\left(-k\, C[0] + \left(k+k^2 - L1\,(1+L1) + Z^2\alpha^2\right) C[1]\right)$ |
| 2 | $2\,E1\,Z\,\alpha\, C[1] + c\,\gamma\,\hbar\left(-(1+k)\, C[1] + \left(2+k\,(3+k) - L1\,(1+L1) + Z^2\alpha^2\right) C[2]\right)$ |
| 3 | $2\,E1\,Z\,\alpha\, C[2] + c\,\gamma\,\hbar\left(-(2+k)\, C[2] + \left(6+k\,(5+k) - L1\,(1+L1) + Z^2\alpha^2\right) C[3]\right)$ |
| 4 | $2\,E1\,Z\,\alpha\, C[3] + c\,\gamma\,\hbar\left(-(3+k)\, C[3] + \left(12+k\,(7+k) - L1\,(1+L1) + Z^2\alpha^2\right) C[4]\right)$ |
| 5 | $2\,E1\,Z\,\alpha\, C[4] + c\,\gamma\,\hbar\left(-(4+k)\, C[4] + \left(20+k\,(9+k) - L1\,(1+L1) + Z^2\alpha^2\right) C[5]\right)$ |

## Determination of recursion formula

$$\text{rule3} = \left\{w \to \left(\sum_{s=q-3}^{q+3} C[s]\, \#^{s+k}\ \&\right)\right\};$$

$$\text{eq5} = \frac{\text{eq3}}{\rho^{-3+k+q}}\ \text{/. rule3 // Expand;}$$

```
list2 = Table[{s, Coefficient[eq5, ρ, s]}, {s, 2, 7}] // Simplify;
list2 // TableForm
```

| | |
|---|---|
| 2 | $(2\,E1\,Z\,\alpha - c\,(-2+k+q)\,\gamma\,\hbar)\, C[-2+q] + c\left(2+k^2 - L1 - L1^2 - 3\,q + q^2 + k\,(-3+2\,q) + Z^2\alpha^2\right)\gamma\,\hbar\, C[-1+q]$ |
| 3 | $(2\,E1\,Z\,\alpha - c\,(-1+k+q)\,\gamma\,\hbar)\, C[-1+q] + c\left(k^2 - L1 - L1^2 - q + q^2 + k\,(-1+2\,q) + Z^2\alpha^2\right)\gamma\,\hbar\, C[q]$ |
| 4 | $(2\,E1\,Z\,\alpha - c\,(k+q)\,\gamma\,\hbar)\, C[q] + c\left(k+k^2 - L1 - L1^2 + q + 2\,k\,q + q^2 + Z^2\alpha^2\right)\gamma\,\hbar\, C[1+q]$ |
| 5 | $(2\,E1\,Z\,\alpha - c\,(1+k+q)\,\gamma\,\hbar)\, C[1+q] + c\left(2+k^2 - L1 - L1^2 + 3\,q + q^2 + k\,(3+2\,q) + Z^2\alpha^2\right)\gamma\,\hbar\, C[2+q]$ |
| 7 | $(2\,E1\,Z\,\alpha - c\,(3+k+q)\,\gamma\,\hbar)\, C[3+q]$ |

```
eq6 = list2[[3, 2]]
```

$$(2\,E1\,Z\,\alpha - c\,(k+q)\,\gamma\,\hbar)\, C[q] + c\left(k+k^2 - L1 - L1^2 + q + 2\,k\,q + q^2 + Z^2\alpha^2\right)\gamma\,\hbar\, C[1+q]$$

```
Solve[eq6 == 0, C[q + 1]]
```

$$\left\{\left\{C[1+q] \to -\frac{(2\,E1\,Z\,\alpha - c\,k\,\gamma\,\hbar - c\,q\,\gamma\,\hbar)\, C[q]}{c\left(k+k^2 - L1 - L1^2 + q + 2\,k\,q + q^2 + Z^2\alpha^2\right)\gamma\,\hbar}\right\}\right\}$$

Determination of k from the first term of the series expansion

```
s1 = (-k + k^2 - L1 - L1^2 + Z^2 α^2); s11 = Solve[s1 == 0, k] // Simplify
```

$$\left\{\left\{k \to \frac{1}{2}\left(1 - \sqrt{1 + 4\,L1 + 4\,L1^2 - 4\,Z^2\alpha^2}\right)\right\}, \left\{k \to \frac{1}{2}\left(1 + \sqrt{1 + 4\,L1 + 4\,L1^2 - 4\,Z^2\alpha^2}\right)\right\}\right\}$$

```
kp = k /. s11[[2]]; km = k /. s11[[1]];
```

We choose kp as k. Determination of the energy eigenvalue under the condition that $C[1+q] = -\frac{(2\,E1\,Z\,\alpha - k\,\gamma - q\,\gamma)\, C[q]}{\left(k+k^2 - L1 - L1^2 + q + 2\,k\,q + q^2 + Z^2\alpha^2\right)\gamma}$ =0 when q=nr (integer)

```
s2p = (2 E1 Z α - c ħ (k γ + q γ)) /. {q → nr} //. {γ → 2/(c ħ) Sqrt[m^2 c^4 - E1^2]} // FullSimplify
```

$$-2\left(\sqrt{-E1^2+c^4 m^2}\ (k+nr)-E1\, Z\, \alpha\right)$$

```
s3 = Solve[s2p == 0, E1] // FullSimplify
```

$$\left\{\left\{E1\to -\frac{c^2 m\ (k+nr)}{\sqrt{(k+nr)^2+Z^2\alpha^2}}\right\},\ \left\{E1\to \frac{c^2 m\ (k+nr)}{\sqrt{(k+nr)^2+Z^2\alpha^2}}\right\}\right\}$$

nr=n-(l+1); principal quantum number

```
s4 = E1 /. s3[[2]] /. {k → kp} /. nr → (n - L1 - 1) // Simplify
```

$$\frac{c^2 m\left(-1-2\,L1+2\,n+\sqrt{1+4\,L1+4\,L1^2-4\,Z^2\alpha^2}\right)}{2\sqrt{Z^2\alpha^2+\frac{1}{4}\left(-1-2\,L1+2\,n+\sqrt{1+4\,L1+4\,L1^2-4\,Z^2\alpha^2}\right)^2}}$$

```
Series[s4, {α, 0, 7}] // Simplify[#, {(-1 - 2 L1 + Sqrt[(1 + 2 L1)^2] + 2 n) > 0, L1 > 0}] &
```

$$c^2 m-\frac{\left(c^2 m Z^2\right)\alpha^2}{2\,n^2}+\frac{c^2 m\ (3+6\,L1-8\,n)\ Z^4\alpha^4}{8\ (1+2\,L1)\ n^4}-\frac{\left(c^2 m\left(5+40\,L1^3+L1^2\ (60-96\,n)-24\,n+24\,n^2+16\,n^3+6\,L1\left(5-16\,n+8\,n^2\right)\right)Z^6\right)\alpha^6}{16\left((1+2\,L1)^3\,n^6\right)}+O[\alpha]^8$$

APPENDIX
Sommerfeld

for an electron of rest mass $m_0$ moving in the Coulomb field of a hydrogen nucleus (Schrödinger did not use the symbol $\hbar$). The equation gave a fine structure for the hydrogen spectrum, but not the correct one. The hydrogen fine structure was first given a theoretical explanation in 1915 by Sommerfeld, who worked with a relativistic extension of Bohr's atomic theory. In his celebrated work, Sommerfeld found that the energy levels of the hydrogen atom were given by the expression

$$W_{n,k} = m_0c^2 \left[ \left(1 + \frac{\alpha^2}{(n - k - \sqrt{k^2 - \alpha^2})^2}\right)^{-\frac{1}{2}} - 1 \right] \qquad (3.5)$$

where $\alpha$ is the fine structure constant (equal to $e/\hbar c$), $n$ the principal quantum number, and $k$ the azimuthal quantum number. Sommerfeld's fine structure formula, or rather its first-order approximation

However, there are reasons to believe that Dirac's retrospection, based on his hope-and-fear moral, is not quite correct. When he created the theory, he was guided by a strong belief in formal beauty and had every reason to be confident that his theory was true. It seems unlikely that he really would have feared that the theory might break down when applied to the hydrogen atom. After all, the Sommerfeld formula had never been tested beyond its first or second approximation; if relativistic quantum mechanics did not reproduce that formula exactly, it could justifiably be argued that it was not exactly true. Dirac's hurry in publication may have been motivated simply by competition, the fear of not being first to publish. Several other physicists were working hard to construct a relativistic spin theory, a fact of which Dirac must have been aware. Naturally he felt that the credit belonged to him. He did not want to be beaten in the race, a fate he had experienced several times already. If agreement with the fine structure formula had the crucial importance that Dirac later asserted, one would expect that he would have attempted to derive the exact fine structure after he submitted his paper for publication. He did not. I think Dirac was quite satisfied with the approximate agreement and had full confidence that his theory would also provide an exact agreement. He simply did not see any point in engaging in the complicated mathematical analysis required for the exact solution.

Other physicists who at the time tried to construct a relativistic spin theory included Hendrik Kramers in Utrecht; Eugene Wigner and Pascual Jordan in Göttingen; and Yakov Frenkel, Dmitri Iwanenko, and Lev Landau in Leningrad. Kramers obtained an approximate quantum description of a relativistic spinning electron in terms of a second-order wave equation and later proved that his equations were equivalent to Dirac's equation. When he got news of Dirac's theory, he was deeply disappointed, and this feeling evolved into a continuing frustration with regard to Dirac's physics. It is unknown in what direction Jordan and Wigner worked (they never published their work), but it seems to have been toward a relativistic extension of Pauli's spin theory. "We were very near to it," Jordan is supposed to have said, "and I cannot forgive myself that I didn't see that the point was linearization."[38] Although disappointed, Jordan recognized the greatness of Dirac's work. "It would have been better had we found the equation but the derivation is so beautiful, and the equation so concise, that we must be happy to have it."[39] Frenkel, Iwanenko, and Landau engaged in laborious tensor calculations and succeeded in working out theories that in some respects were similar to Dirac's. But apart from being published after Dirac's work, they lacked, like Kramers's theory, the beauty and surprising simplicity that characterized Dirac's theory.[40] Still, there can be little doubt that had Dirac not published his theory in January 1928, an equivalent theory would have been published by other physicists within a few months. Dirac later said that if he had not obtained the wave equation of the electron, Kramers would have.[41]