Phys 483 / Fall 2002

HW II Solution

1. $\psi(\vec{r},t) = \frac{1}{r} R_\ell(r) Y_{\ell m}(\theta,\phi) \exp(-\frac{i}{\hbar}\epsilon t)$,

where $R_\ell(r)$ obeys K-G eq:

$$\left[\frac{d^2}{dr^2} - \frac{\lambda(\lambda+1)}{r^2} + \frac{2\epsilon Z\alpha}{\hbar c r} - \frac{(mc^2)^2-\epsilon^2}{\hbar^2 c^2} \right] R_\ell(r) = 0,$$

with $\lambda = -\frac{1}{2} + \sqrt{(\ell+\frac{1}{2})^2 - (Z\alpha)^2}$, and $\alpha = \frac{e^2}{\hbar c}$ being the fine structure constant.

(a) Introduce the scaled radial coordinate,

$$\rho = 2\frac{\sqrt{(mc^2)^2-\epsilon^2}}{\hbar c} r = \beta r.$$

$$\frac{d}{dr} = \frac{d}{d\rho}\frac{d\rho}{dr} = \beta\frac{d}{d\rho}, \quad \frac{d^2}{dr^2} = \beta^2\frac{d^2}{d\rho^2}$$

$$\frac{1}{r} = \frac{\beta}{\rho}, \quad \frac{1}{r^2} = \frac{\beta^2}{\rho^2}.$$

Rewrite KG eq in ρ:

$$\left[\beta^2\frac{d^2}{d\rho^2} - \beta^2\frac{\lambda(\lambda+1)}{\rho^2} + \beta\frac{2\epsilon Z\alpha}{\hbar c\rho} - \frac{(mc^2)^2-\epsilon^2}{\hbar^2 c^2} \right] R_\ell(\rho) = 0$$

Divide β^2 on both sides:

$$\left[\frac{d^2}{d\rho^2} - \frac{\lambda(\lambda+1)}{\rho^2} + \frac{1}{\beta}\frac{2\epsilon Z\alpha}{\hbar c\rho} - \frac{1}{\beta^2}\frac{(mc^2)^2-\epsilon^2}{\hbar^2c^2}\right] R_\ell(\rho) = 0$$

$$\frac{1}{\beta}\frac{2Z\epsilon\alpha}{\hbar c} = \frac{\cancel{\hbar c}}{\cancel{2}\sqrt{(mc^2)^2-\epsilon^2}} \cdot \frac{\cancel{2}\epsilon Z\alpha}{\cancel{\hbar c}} = \frac{Z\alpha\epsilon}{\sqrt{(mc^2)^2-\epsilon^2}}$$

$$\frac{1}{\beta^2}\frac{(mc^2)^2-\epsilon^2}{\hbar^2c^2} = \frac{\cancel{\hbar^2c^2}}{4\cancel{[(mc^2)^2-\epsilon^2]}}\frac{\cancel{(mc^2)^2-\epsilon^2}}{\cancel{\hbar^2c^2}} = \frac{1}{4}$$

By definition $\nu \equiv \dfrac{Z\alpha\epsilon}{\sqrt{(mc^2)^2-\epsilon^2}}$, the differential equation is now:

$$\boxed{\left[\frac{d^2}{d\rho^2} - \frac{\lambda(\lambda+1)}{\rho^2} + \frac{\nu}{\rho} - \frac{1}{4}\right] R_\ell(\rho) = 0}$$

(b) In analogy to the case of stationary bound states for the non-relativistic hydrogen atom, let's first investigate $R_\ell(\rho)$ as $\rho \to 0$ and $\rho \to \infty$.

1) As $\rho \to \infty$, the leading term is $-\frac{1}{4}$.

$$\left(\frac{d^2}{d\rho^2} - \frac{1}{4}\right) R_\ell(\rho) = 0 \implies R_\ell(\rho) \sim e^{\pm\frac{\rho}{2}}.$$

We drop the "+" solution since it diverges.

$$R_\ell(\rho) \sim e^{-\frac{1}{2}\rho}$$

2) As $\rho \to 0$, the leading term is $-\frac{\lambda(\lambda+1)}{\rho^2}$.

$$\left[\frac{d^2}{d\rho^2} - \frac{\lambda(\lambda+1)}{\rho^2}\right] R_\ell(\rho) = 0$$

$$R_\ell(\rho) \sim \rho^{\lambda+1} \quad \text{or} \quad R_\ell(\rho) \sim \rho^{-\lambda}$$

Again we take $R_l(\rho) \sim \rho^{\lambda+1}$ from physical considerations.

In general, we can write $R_\ell(\rho)$ as:

$$R_\ell(\rho) = N \rho^{\lambda+1} e^{-\frac{\rho}{2}} \sum_{j=0}^{\infty} a_j \rho^j,$$

where N is a normalization constant.

(c) To avoid the possibility that the polynomial cancels the exponential decay as $\rho \to \infty$, one need to confine j below a finite number n'. It will be clarified further in part (d).

(d) $$R_\ell(\rho) = N\rho^{\lambda+1} e^{-\frac{1}{2}\rho} \sum_{j=0}^{n'} a_j \rho^j$$
$$= N e^{-\frac{1}{2}\rho} \sum_{j=0}^{n'} a_j \rho^{j+\lambda+1}$$

$$\frac{d^2 R_\ell(\rho)}{d\rho^2} = N e^{-\frac{1}{2}\rho} \sum_{j=0}^{n'} a_j \left[\frac{1}{4}\rho^{j+\lambda+1} - (j+\lambda+1)\rho^{j+\lambda} + (j+\lambda+1)(j+\lambda)\rho^{j+\lambda-1} \right]$$

$$\left[\frac{d^2}{d\rho^2} - \frac{\lambda(\lambda+1)}{\rho^2} + \frac{\nu}{\rho} - \frac{1}{4} \right] R_\ell(\rho)$$
$$= N e^{-\frac{1}{2}\rho} \sum_{j=0}^{n'} \left\{ a_j (\nu - j - \lambda - 1)\rho^{j+\lambda} + a_j \left[(j+\lambda+1)(j+\lambda) - \lambda(\lambda+1) \right] \rho^{j+\lambda-1} \right.$$
$$= 0$$

The coefficients of the expansion must vanish. Then we have:

$$a_j(\nu - j - \lambda - 1) + a_{j+1}[(j+\lambda+2)(j+\lambda+1) - \lambda(\lambda+1)] = 0$$

$$a_j(\nu - j - \lambda - 1) + a_{j+1}(j+1)(j+2\lambda+2) = 0 .$$

$$a_{j+1} = \frac{a_j}{j+1}\,\frac{a+j}{b+j}, \quad \text{where } a \equiv \lambda - \nu + 1,\ b \equiv 2\lambda + 2.$$

$$\lim_{j\to\infty} \frac{a_{j+1}}{a_j} = \frac{a+j}{(j+1)(b+j)} \sim \frac{1}{j+1}.$$ This is the same behavior as an exponential function. So n' must be finite.

(e) The condition $a_{n'+1} = 0$ implies:

$$a + n' = \lambda - \nu + 1 + n' = 0$$

Recall the definitions of λ and ν; we have

$$\frac{1}{2} + \sqrt{(l+\tfrac{1}{2})^2 - (Z\alpha)^2} - \frac{\varepsilon Z\alpha}{\sqrt{(mc^2)^2 - \epsilon^2}} + n' = 0 ,$$

which leads to

$$\frac{Z^2\alpha^2\epsilon^2}{(mc^2)^2 - \epsilon^2} = \left[n' + \frac{1}{2} + \sqrt{(l+\tfrac{1}{2})^2 - (Z\alpha)^2}\right]^2 ,$$

and finally

$$\epsilon = mc^2 \frac{1}{\sqrt{1 + \dfrac{Z^2\alpha^2}{\left(n' + \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - (Z\alpha)^2}\right)^2}}}$$

(f) When Z is not very large, i.e. $Z\alpha < 1/2$, the bound state energy can be expanded as powers of $Z\alpha$.

$$\left[(l+\tfrac{1}{2})^2-(Z\alpha)^2\right]^{\frac{1}{2}}=(l+\tfrac{1}{2})\left[1-\frac{1}{2}\left(\frac{Z\alpha}{l+\frac{1}{2}}\right)^2+O(Z\alpha)^4\right]$$

Define $n \equiv n'+l+1$, then

$$n'+\frac{1}{2}+\left[(l+\tfrac{1}{2})^2-(Z\alpha)^2\right]^{\frac{1}{2}}$$

$$= n-\frac{1}{2}\frac{(Z\alpha)^2}{l+\frac{1}{2}}+O(Z\alpha)^4$$

$$\frac{(Z\alpha)^2}{\left(n-\frac{1}{2}\frac{(Z\alpha)^2}{l+\frac{1}{2}}+O(Z\alpha)^4\right)^2}=\frac{(Z\alpha)^2}{\left(n^2-\frac{n}{l+\frac{1}{2}}(Z\alpha)^2+O(Z\alpha)^4\right)}$$

$$=\frac{Z^2\alpha^2}{n^2}+\frac{(Z^2\alpha^2)^2}{n^3(l+\frac{1}{2})}+O(Z^2\alpha^2)^3$$

$$E_{nl}=mc^2\frac{1}{\sqrt{1+\frac{Z^2\alpha^2}{n^2}+\frac{(Z^2\alpha^2)^2}{n^3(l+\frac{1}{2})}+O(Z^2\alpha^2)^3}}$$

$$=mc^2\left[1-\frac{Z^2\alpha^2}{2n^2}-\frac{(Z^2\alpha^2)^2}{2n^4}\frac{n}{l+\frac{1}{2}}+\frac{3}{8}\left(\frac{Z^2\alpha^2}{n^2}\right)^2+O(Z^2\alpha^2)^3\right]$$

$$=mc^2\left[1-\frac{Z^2\alpha^2}{2n^2}-\frac{(Z^2\alpha^2)^2}{2n^4}\left(\frac{n}{l+\frac{1}{2}}-\frac{3}{4}\right)+O(Z^2\alpha^2)^3\right]$$

■ Problem 1 (g):

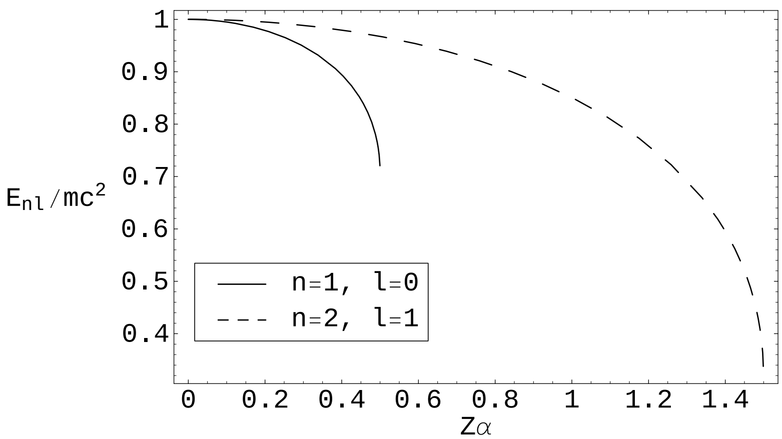
```
<< Graphics`Graphics`
<< Graphics`Legend`

(* First, we use the original energy function.  To  make the  root real,
 z<0.5 for and first case and z<1.5 for the second case are required. *)

nprime[n_, l_] := n - l - 1;
```

$$\text{E0}[n\_, l\_, z\_] := 1 \Big/ \text{Sqrt}\left[1 + \left(\frac{z}{\text{nprime}[n, l] + \frac{1}{2} + \text{Sqrt}\left[\left(l + \frac{1}{2}\right)^2 - z^2\right]}\right)^2\right];$$

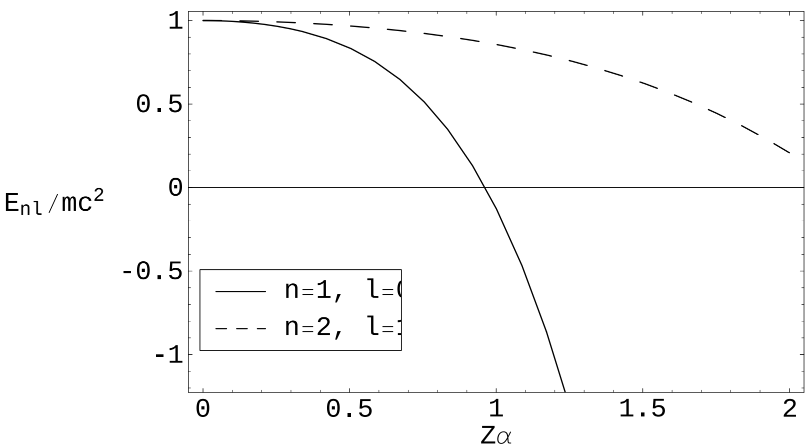
```
Plot[{E0[1, 0, z], E0[2, 1, z]}, {z, 0, 2}, Frame → True, FrameLabel → {"Zα", "E_nl/mc^2"},
  RotateLabel → False, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotLegend → {"n=1, l=0", "n=2, l=1"}, LegendPosition -> {-0.5, -0.3},
  LegendSize -> {0.6, 0.2}, LegendShadow → {0, 0}];
```



```
(* However, if the expansion is used, there is no limitation of Z.
   Thus we see artificial effects. *)
```

$$\texttt{Enl[n\_, l\_, z\_] := } 1 - \frac{z^2}{2\,n^2} - \frac{z^4}{2\,n^4}\left(\frac{n}{l+0.5} - \frac{3}{4}\right);$$

```
Plot[{Enl[1, 0, z], Enl[2, 1, z]},
  {z, 0, 2}, Frame → True, FrameLabel → {"Zα", "E_nl/mc^2"},
  RotateLabel → False, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotLegend → {"n=1, l=0", "n=2, l=1"}, LegendPosition -> {-0.5, -0.3},
  LegendSize -> {0.5, 0.2}, LegendShadow → {0, 0}];
```



■ Problem 1 (h):

```
(* For n=1, l=0, we have n'=0. For n=2, l=1, we still have n'=0 *)
```

$$\alpha = \frac{1}{137};$$

$$\lambda\texttt{[z\_, l\_] := } -\frac{1}{2} + \texttt{Sqrt}\left[\left(l + \frac{1}{2}\right)^2 - (z\,\alpha)^2\right];$$

$$\texttt{RDirac[z\_, l\_, }\rho\texttt{\_] := }\rho^{\lambda[z,l]+1}\,\texttt{Exp}\left[-\frac{\rho}{2}\right];$$

$$\texttt{RSdg[l\_, }\rho\texttt{\_] := }\rho^{l+1}\,\texttt{Exp}\left[-\frac{\rho}{2}\right];$$

```
(* The radial part of wave functions are actually ρ*RDirac[z,l,ρ] and ρ*RSdg[l,ρ].
    To avoid divergence at ρ=0, we plot RDirac and RSdg here. *)
```

```
{N[λ[1, 0]], N[λ[50, 0]]}
```

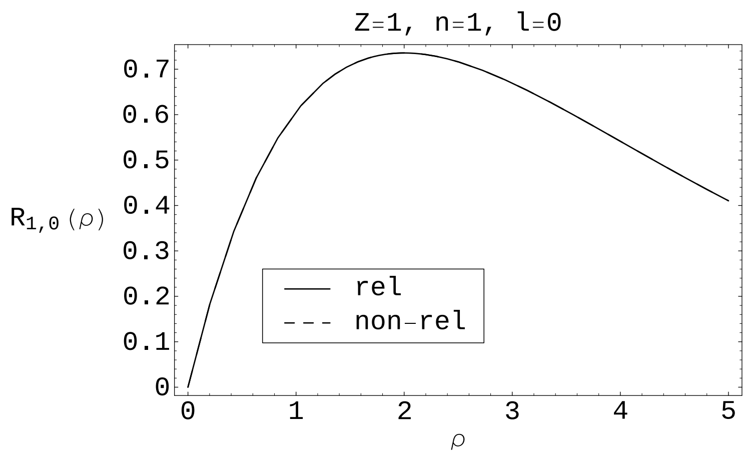
```
{-0.0000532822, -0.158237}
```

```
{N[λ[1, 1]], N[λ[50, 1]]}
```

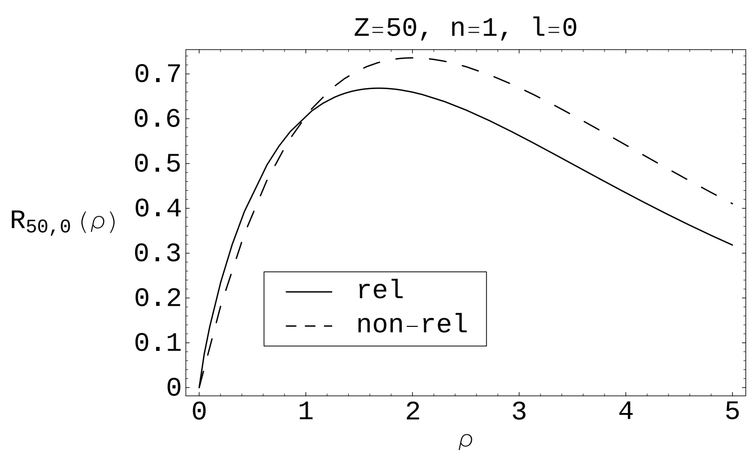
```
{0.999982, 0.954923}
```

```
(* As Z=1, Zα <<1, and λ≃l,
 we then expect little vavriation of R. When Zα get larger,
 the relativistic and non-
  relativistic functions look more different. From problem 1 (g),
 we know that λ becomes a complex number when Zα>0.5 for n=1,
 l=0 and Zα>1.5 for n=2,
 l=1. At Z=50, Zα=0.364, the difference is more pronounced for n=1 and  l=0 case. *)
```

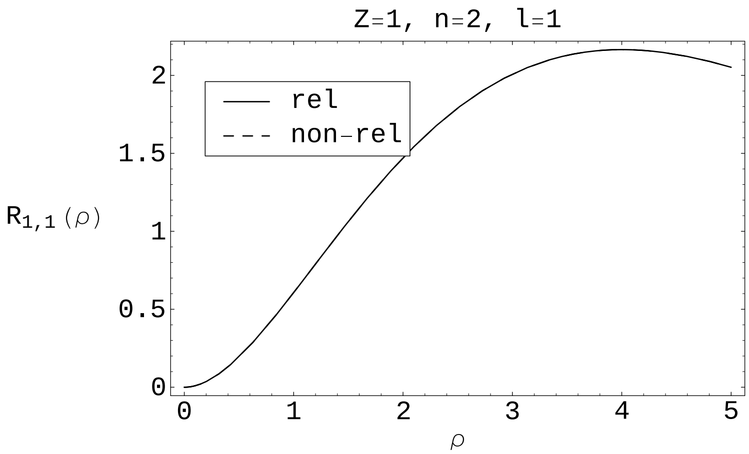
```
Plot[{RDirac[1, 0, x], RSdg[0, x]},
  {x, 0, 5}, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotRange → All, PlotLabel → "Z=1, n=1, l=0",
  Frame → True, FrameLabel → {"ρ", "R1,0(ρ)"},
  RotateLabel → False, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotLegend → {"rel", "non-rel"}, LegendPosition -> {-0.3, -0.3},
  LegendSize -> {0.6, 0.2}, LegendShadow → {0, 0}];
```




```
Plot[{RDirac[50, 0, x], RSdg[0, x]},
  {x, 0, 5}, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotRange → All, PlotLabel → "Z=50, n=1, l=0",
  Frame → True, FrameLabel → {"ρ", "R50,0(ρ)"},
  RotateLabel → False, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotLegend → {"rel", "non-rel"}, LegendPosition -> {-0.3, -0.3},
  LegendSize -> {0.6, 0.2}, LegendShadow → {0, 0}];
```



```
Plot[{RDirac[1, 1, x], RSdg[1, x]},
  {x, 0, 5}, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotRange → All, PlotLabel → "Z=1, n=2, l=1",
  Frame → True, FrameLabel → {"ρ", "R1,1(ρ)"},
  RotateLabel → False, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotLegend → {"rel", "non-rel"}, LegendPosition -> {-0.45, 0.2},
  LegendSize -> {0.55, 0.2}, LegendShadow → {0, 0}];
```




```
Plot[{RDirac[50, 1, x], RSdg[1, x]},
  {x, 0, 5}, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotRange → All, PlotLabel → "Z=50, n=2, l=1",
  Frame → True, FrameLabel → {"ρ", "R20,1(ρ)"},
  RotateLabel → False, PlotStyle → {GrayLevel[0], Dashing[{.03}]},
  PlotLegend → {"rel", "non-rel"}, LegendPosition -> {-0.45, 0.2},
  LegendSize -> {0.55, 0.2}, LegendShadow → {0, 0}];
```