Notes for Dark Photon Sensitivity Calculation

Joonseok Hur

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1 Units of length and energy

To solve wavefunctions length and energy are to be normalized. Normalized quantities will have tilde on it in this document. For atomic physics Bohr radius $a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = 52.917721067(12)$ pm is useful as length scale.

$$\tilde{\mathbf{r}} \equiv \mathbf{r}/a_0 \tag{1}$$

Then derivative with respect to coordinate is given as

$$\tilde{\nabla} = a_0 \nabla \tag{2}$$

in the sense that.

$$\frac{\partial}{\partial\tilde{\mathbf{r}}}\bar{f}(\mathbf{r}) = a_0 \frac{\partial}{\partial(a_0\tilde{\mathbf{r}})}\bar{f}(a_0\tilde{\mathbf{r}}) = a_0 \frac{\partial}{\partial\mathbf{r}}f(\mathbf{r}) \tag{3}$$

where $\bar{f}(\tilde{\mathbf{r}}) = f(a_0\tilde{\mathbf{r}})$ is a function with normalized argument. Bars on functions will be omitted for the rest of this document unless there are ambiguities.

Note that Bohr radius a_0 can be express as follows in the context of high-energy physics:

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} = \frac{\hbar}{m_e c\alpha} = \frac{\lambda_e}{\alpha} \tag{4}$$

where $\alpha = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c} = 1/137.035999139(31)$ is fine-structure constant, m_e is rest mass of electron, and $\lambda_e = \frac{\hbar}{m_e c}$ is reduced Compton wavelength of electron.

On the other hand, There are two relevant units for energy. Atomic physics would prefer Hartree ($E_{\mathrm{h}} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{a_0}$; potential energy of electron in the ground state of (infinite proton-mass) hydrogen $= \frac{\hbar c\alpha}{a_0} = \alpha^2 m_e c^2$), while in high-energy physics the unit of energy (or mass) would be inverse of length by expressing energy in the form of (reduced) Compton wavelength $\lambda_E = \frac{\hbar c}{E}$ (or, for mass, $\lambda_m = \frac{\hbar}{mc}$). Interestingly, combining length in Bohr radius and energy in inverse length gives a relevant energy scale in atomic physics as follows.

$$\tilde{E} \equiv \frac{a_0}{\lambda_E} = \frac{a_0}{\hbar c}E = \frac{E}{E_0} \tag{5}$$

where

$$
\begin{aligned}
E_0 &= \frac{\hbar c}{a_0} = \frac{E_{\mathrm{h}}}{\alpha} = \alpha m_e c^2 \\
&= 3.7289394707275227(??) \text{ keV} \\
&= 0.3324919 \text{ nm} \\
&= 901\ 653.5 \text{ THz} \\
&\approx 270 \times \text{Rydberg frequency } (= 3.289841960410^1 5 \text{ Hz})
\end{aligned}
\tag{6}
$$

The last two term in energy unit E_0 manifest its usefulness in atomic physics in high-energy physics, respectively. For mass,

$$
\tilde{m} \equiv \frac{a_0}{\lambda_m} = \frac{m}{m_0}
\tag{7}
$$

where

$$
m_0 = \alpha m_e = 4.0031810073274429 \times 10^{-6} u
\tag{8}
$$

As examples, Coulomb potential energy as a function of r can be normalized as follows:

$$
\tilde{V}(\tilde{r}) = \frac{V(r)}{E_0} = \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \frac{a_0}{\hbar c} = \frac{Z\alpha}{\tilde{r}}
\tag{9}
$$

and mass of electron is just inverse of fine-structure constant ($\tilde{m}_e = 1/\alpha \sim 137$).

2 Schrödinger equation

By dividing Schrödinger equation

$$
-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r})\xi(\mathbf{r}) = E\psi(\mathbf{r})
\tag{10}
$$

with E_0 one gets

$$
-\frac{1}{2\tilde{m}} \tilde{\nabla}^2 \psi(\tilde{\mathbf{r}}) + \tilde{V}(\mathbf{r})\tilde{\psi}(\tilde{\mathbf{r}}) = \tilde{E}\psi(\tilde{\mathbf{r}})
\tag{11}
$$

If a potential is isotropic ($V(\mathbf{r}) = V(r)$) one can use a separation of variables $\psi(\mathbf{r}) = R(r)Y_l^m(\theta, \phi)$ and equation for radial wavefunction $R(r)$ is given as

$$
-\frac{\hbar^2}{2mr} \frac{d^2}{dr^2}[rR(r)] + \left[\frac{\hbar^2 l(l+1)}{2mr^2} + V(r) \right] R(r) = ER(r)
\tag{12}
$$

Again, by dividing above with E_0 and multiply $2\tilde{m}\tilde{r}$ one gets

$$
-\frac{d^2}{d\tilde{r}^2} u(\tilde{r}) + \left[\frac{l(l+1)}{\tilde{r}^2} + 2\tilde{m}\tilde{V}(\tilde{r}) \right] u(\tilde{r}) = 2\tilde{m}\tilde{E}u(\tilde{r})
\tag{13}
$$

where $u(\tilde{r}) = \tilde{r}R(\tilde{r})$. The above differential equation is to be used for calculating radial wavefunctions. Normalization condition is given as

$$
1 = \int_0^\infty r^2 dr \int d\Omega \, |R(r)Y_l^m(\theta,\phi)|^2 = \int_0^\infty dr r^2 R(r)^2 = \int_0^\infty dr u(r)^2
\tag{14}
$$

2

3   Thomas-Fermi potential

Thomas-Fermi potential is used for calculating potential of core in n-th ionized ion with atomic number Z including screening effect of core electrons:

$$V_{TF}(r) = \begin{cases} -\frac{1}{4\pi\epsilon_0}\left[\frac{Ze^2}{r}\chi\left(4\sqrt[3]{\frac{2Z}{9\pi^2}}\frac{r}{a_0}\right) - \frac{ne^2}{r_0}\right] & r \leq r_0 \\ -\frac{1}{4\pi\epsilon_0}\frac{ne^2}{r} & r > r_0 \end{cases} \tag{15}$$

where $\chi(x)$ is a function which satisfy

$$\frac{d^2\chi}{dx^2} = \sqrt{\frac{\chi^3}{x}} \tag{16}$$

with conditions $\chi(0) = 1$, $\chi(x_0) = 0$, $x_0\chi'(x_0) = -n/Z$ for an x_0, and $4\sqrt[3]{\frac{2Z}{9\pi^2}}\frac{r_0}{a_0} = x_0$. One can imagine that, from boundary conditions at $x = 0$ and $x = x_0$, $\chi(x)$ will change from 1 to 0 as x goes from 0 to 1 and $V_{TF}(r)$ would shows smooth transition from unscreened potential $-\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}$ to screened potential $-\frac{1}{4\pi\epsilon_0}\frac{ne^2}{r}$ at $r \leq r_0$. After normalization,

$$\tilde{V}_{TF}(r) = \begin{cases} \frac{Z\alpha^2}{\tilde{r}}\chi\left(4\sqrt[3]{\frac{2Z}{9\pi^2}}\tilde{r}\right) - \frac{n\alpha^2}{\tilde{r}_0} & \tilde{r} \leq \tilde{r}_0 \\ \frac{n\alpha^2}{\tilde{r}} & \tilde{r} > \tilde{r}_0 \end{cases} \tag{17}$$

where $4\sqrt[3]{\frac{2Z}{9\pi^2}}\tilde{r}_0 = x_0$.

For our calculation, nuclear potential from Helm charge distribution model may be used as unscreened potential, instead of $-\frac{Z\alpha}{\tilde{r}}$ in Thomas-Fermi potential (See Fig.1):

$$\tilde{V}(r) = \begin{cases} \tilde{V}_{\text{Helm}}(\tilde{r})\chi\left(4\sqrt[3]{\frac{2Z}{9\pi^2}}\tilde{r}\right) - \frac{n\alpha^2}{\tilde{r}_0} & \tilde{r} \leq \tilde{r}_0 \\ \frac{n\alpha^2}{\tilde{r}} & \tilde{r} > \tilde{r}_0 \end{cases} \tag{18}$$

4   Radial Dirac equation

For Dirac equation:

$$\tilde{H}\Psi(\tilde{x}^\beta) = \left[-i\tilde{\not{\partial}} + \tilde{m} + \gamma^0\tilde{V}(\tilde{r})\right]\Psi(\tilde{x}^\beta) \tag{19}$$

(clarifier: $\tilde{V}(\tilde{r}) \equiv V(a_0\tilde{r})/E_0 = -Z\alpha/\tilde{r}$ for Hydrogen-like atom), an ansatz

$$\Psi(\tilde{x}^\beta) = e^{-i\tilde{E}\tilde{t}}\Psi(\tilde{\mathbf{x}}) = e^{-i\tilde{E}\tilde{t}}\begin{pmatrix} \phi(\tilde{\mathbf{x}}) \\ \chi(\tilde{\mathbf{x}}) \end{pmatrix} \tag{20}$$

(Proper normalization of time would be $\tilde{t} = ct/a_0$) gives

$$\begin{aligned} \left(\tilde{E} - \tilde{V}(a_0\tilde{r}) - \tilde{m}\right)\phi(\tilde{\mathbf{x}}) &= -i\sigma\tilde{\nabla}\chi(\tilde{\mathbf{x}}) \\ \left(\tilde{E} - \tilde{V}(a_0\tilde{r}) + \tilde{m}\right)\chi(\tilde{\mathbf{x}}) &= -i\sigma\tilde{\nabla}\phi(\tilde{\mathbf{x}}) \end{aligned} \tag{21}$$

and

$$\phi_{nk}(\tilde{\mathbf{x}}) = \frac{g_{nk}(\tilde{r})}{\tilde{r}}\Omega_{km}(\theta, \phi), \quad \chi_{nk}(\tilde{\mathbf{x}}) = \frac{if_{nk}(\tilde{r})}{\tilde{r}}\Omega_{-km}(\theta, \phi) \tag{22}$$
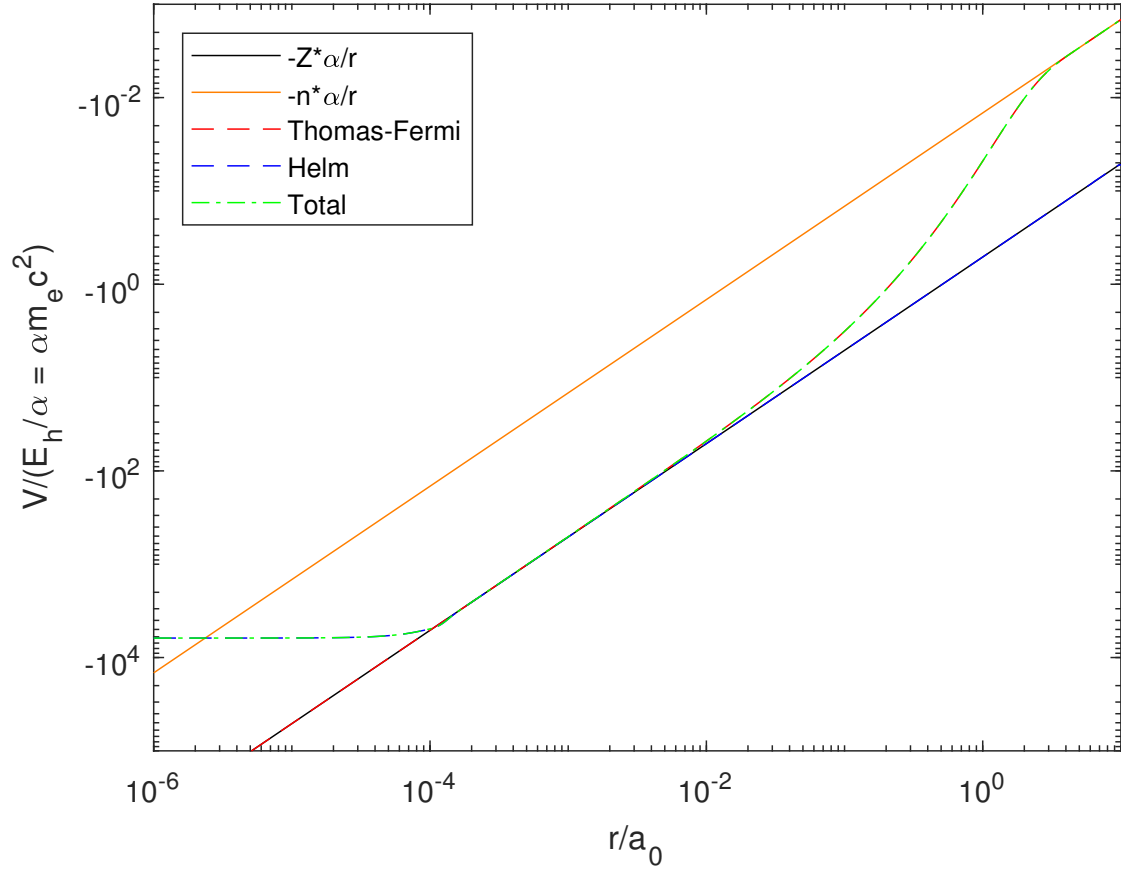
3

Figure 1: Comparison of relevant potentials for Yb+ ($Z = 70$, $n = 2$). Total potential is to be used for calculation.

is an ansatz of it, where Ω is Weyl spinor and quantum number k is given as

$$k = \mp \left(j + \frac{1}{2} \right) = \begin{cases} -l - 1, & j = l + 1/2 \\ l, & j = 1 - 1/2 \end{cases} \tag{23}$$

for given total angular momentum quantum number. One can see that $f(\tilde{r})$, $g(\tilde{r})$ correspond to $\tilde{r}R(\tilde{r}) = U(\tilde{r})$ in non-relativistic case and so $\Omega_{km}(\theta, \phi)$ does to Y_{lm} with the relation between k and l. We have interest in radial parts $g(\tilde{r})$ and $f(\tilde{r})$ only, and equations for them (radial Dirac equations) are given as

$$\partial_{\tilde{r}} \begin{pmatrix} g \\ f \end{pmatrix} = \begin{pmatrix} -\frac{k}{\tilde{r}} & -\tilde{E} + \tilde{V}(\tilde{r}) - \tilde{m} \\ \tilde{E} - \tilde{V}(\tilde{r}) - \tilde{m} & \frac{k}{\tilde{r}} \end{pmatrix} \begin{pmatrix} g \\ f \end{pmatrix} \tag{24}$$

In fact, there is more rigorous treatment of two-body problem. The equation above seems to be exact only in the case of infinite nucleus.

Numerical solution could be achieved in two ways. The equation could be arranged to be an eigenproblem:

$$\begin{pmatrix} \tilde{V}(\tilde{r}) + \tilde{m} & -\partial_{\tilde{r}} - \frac{k}{\tilde{r}} \\ \partial_{\tilde{r}} - \frac{k}{\tilde{r}} & \tilde{V}(\tilde{r}) - \tilde{m} \end{pmatrix} \begin{pmatrix} g' \\ f \end{pmatrix} = \tilde{E} \begin{pmatrix} g' \\ f \end{pmatrix} \tag{25}$$

with substitution $g'(\tilde{r}) = -g(\tilde{r})$, or one can put one equation to another and get second-order differential equation. Unfortunatly, the resulting differential equation in the second approach doesn't seem to be able to be rearranged to be an eigenproblem. For the first approach, it would be better to stagger coordinates of g and f [i.e, $(g_1, f_1, g_2, f_2, ..., g_N, f_N)$] instead of following the expression in the equation $(\mathbf{g}, \mathbf{f})$, to make matrix to be diagonalized as diagonal as possible.

$$dd \tag{26}$$

5 Hydrogen atom

The (nonrelativistic) radial wavefunction of an electron in (infinite-mass) Hydrogen-like atom under potential $V(r) = \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r}$ (or $\tilde{V}(\tilde{r}) = \frac{Z\alpha}{\tilde{r}}$) is given as

$$R_{nl}(r) = \sqrt{\left(\frac{2Z}{na_0} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]}} e^{-Zr/na_0} \left(\frac{2Zr}{na_0} \right)^l L_{n-l-1}^{2l+1} \left(\frac{2Zr}{na_0} \right) \tag{27}$$

or

$$R_{nl}(\tilde{r}) = \sqrt{\left(\frac{2Z}{n} \right)^3 \frac{(n-l-1)!}{2n[(n+l)!]}} e^{-Z\tilde{r}/n} \left(\frac{2Z\tilde{r}}{n} \right)^l L_{n-l-1}^{2l+1} \left(\frac{2Z\tilde{r}}{n} \right) \tag{28}$$

where L_{n-l-1}^{2l+1} is the generalized Laguerre polynomial of degree $n - l - 1$, with energy

$$E_n = -\frac{m_e e^4}{(4\pi\epsilon_0)^2 \hbar^2} \frac{Z^2}{2n^2} = \alpha^2 m_e c^2 \frac{Z^2}{2n^2}, \quad \tilde{E}_n = -\frac{Z^2\alpha}{2n^2} \tag{29}$$

5

The Dirac radial wavefunctions in

$$\Phi(\tilde{r}, \theta, \phi) = \begin{pmatrix} \frac{g_{nk}(\tilde{r})}{\tilde{r}} \Omega_{km}(\theta, \phi) \\ \frac{if_{nk}(\tilde{r})}{\tilde{r}} \Omega_{-km}(\theta, \phi) \end{pmatrix} \tag{30}$$

are given as

$$\begin{pmatrix} g_{nk}(\tilde{r}) \\ f_{nk}(\tilde{r}) \end{pmatrix} = \frac{1}{\sqrt{2k(k-\gamma)}} \begin{pmatrix} Z\alpha & -(k-\gamma) \\ -(k-\gamma) & Z\alpha \end{pmatrix} \begin{pmatrix} u_{nk}^+(\tilde{r}) \\ u_{nk}^-(\tilde{r}) \end{pmatrix} \tag{31}$$

where

$$\begin{pmatrix} u_{nk}^+(\tilde{r}) \\ u_{nk}^-(\tilde{r}) \end{pmatrix} = (2C_{nk}\tilde{r})^\gamma e^{-C_{nk}\tilde{r}} \begin{pmatrix} \tilde{\mathcal{A}}_{+,nk} 2\tilde{C}_{nk}\tilde{r} L_{n_r-1}^{2\gamma+1}(2\tilde{C}_{nk}\tilde{r}) \\ \tilde{\mathcal{A}}_{-,nk} L_{n_r}^{2\gamma-1}(2\tilde{C}_{nk}\tilde{r}) \end{pmatrix} \tag{32}$$

$$\tilde{\mathcal{A}}_{+,nk} = \begin{cases} 0, & n_r = 0 \\ \sqrt{\frac{\tilde{C}_{nk}(n_r-1)!}{\Gamma(n_r+2\gamma+1)}} \frac{n_r+\gamma+\frac{\gamma}{k}\sqrt{Z^2\alpha^2+(n_r+\gamma)^2}}{2\frac{\gamma^2}{k^2}(Z^2\alpha^2+(n_r+\gamma)^2)}, & n_r > 0 \end{cases}$$

$$\tilde{\mathcal{A}}_{-,nk} = \sqrt{\frac{\tilde{C}_{nk}n_r!}{\Gamma(n_r+2\gamma)}} \frac{n_r+\gamma-\frac{\gamma}{k}\sqrt{Z^2\alpha^2+(n_r+\gamma)^2}}{2\frac{\gamma^2}{k^2}(Z^2\alpha^2+(n_r+\gamma)^2)} \tag{33}$$

$$\tilde{E}_{nk} = \frac{\tilde{m}_e}{\sqrt{1+\frac{Z^2\alpha^2}{(n_r+\gamma)^2}}} = \frac{1}{\alpha\sqrt{1+\frac{Z^2\alpha^2}{(n_r+\gamma)^2}}}$$

$$\tilde{C}_{nk} = \sqrt{\tilde{m}_e^2 - \tilde{E}_{nk}^2} = \sqrt{1/\alpha^2 - \tilde{E}_{nk}^2} \tag{34}$$

$$\gamma = \sqrt{k^2 - Z^2\alpha^2}$$

and

$$n_r = n - |k|, \quad k = \mp\left(j + \tfrac{1}{2}\right) = \begin{cases} -l-1, & j = l+1/2 \\ l, & j = 1-1/2 \end{cases} \tag{35}$$

given that $\tilde{m} = 1/\alpha$ as shown previously. Probability density over r is given as

$$P(\tilde{r}) = f^2(\tilde{r}) + g^2(\tilde{r}) \tag{36}$$

Be careful. $P(\tilde{r})$ does not mean probability density at a *point* distant from origin by $\tilde{r}$. It rather mean that there are probability of $P(\tilde{r})d\tilde{r}$ being in a spherical shell between $(\tilde{r}, \tilde{r}+d\tilde{r})$. The proper normalization is, therefore, $1 = \int_0^\infty d\tilde{r}P(\tilde{r})$ rather than $1 = \int_0^\infty \tilde{r}^2 d\tilde{r}P(\tilde{r})$.

6 To be continued...

7 Appendix: Value of constants

Fine-structure constant $\alpha = 0.0072973525664(17) = 1/137.035999139(31)$

Reduced plank constant $\hbar = 1.054571800(13) \times 10^{34}$ J·s $= 4.135667662(25)1015$ eV·s

$\hbar c = 0.19732697$ eV·μm

Electron rest mass $m_e = 9.10938356(11) \times 10^{31}$ kg $= 5.48579909070(16) \times 10^4$ u $= 0.5109989461(31)$ MeV/c^2

Bohr radius $a_0 = 5.2917721067(12) \times 10^{11}$ m

Hartree $E_{\rm h} = 27.21138602(17)$ eV