❦ Complementary Homework TIF290 ❦

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1 Problem 3 ass #3

We found in the lecture that the canonical momentum is no longer mass times velocity. This may raise a question about the probability flux: does the probability flux involve the canonical momentum or the kinematic momentum? I ask you to derive the probability flux for a charged particle in a magnetic field/vector potential. Write the result with only wavefunctions and either the canonical or the kinematic momentum. Then prove that the probability flux is gauge invariant.

1.1 Solution

We consider this problem in the position basis. Let $\hbar = c = q = 1$.

We first make a qualified guess for how the probability flux looks in an EM field by replacing the canonical momentum $\vec{p}$ with the kinematic momentum $\vec{\pi} = \vec{p} - \vec{A}$ in the previous, non-EM, definition:

$$\vec{\jmath} = \frac{1}{2m}\left[\psi^* \vec{\pi}\psi + \psi(\vec{\pi}\psi)^*\right]. \tag{1}$$

We now want to show that this definition satisfies the continuity equation

$$\partial_t \rho + \vec{\nabla} \cdot \vec{\jmath} = 0. \tag{2}$$

Firstly,

$$\begin{aligned}
\partial_t \rho &= (\partial_t \psi)\psi^* + \psi(\partial_t \psi^*) \\
&\overset{\text{S.E.}}{=} (-iH\psi)\psi^* + \psi(-iH\psi)^* \\
&= -\psi^* i(\frac{1}{2m}\vec{\pi}^2 + \phi)\psi + \psi i\big((\frac{1}{2m}\vec{\pi}^2 + \phi)\psi\big)^* \\
&\overset{\phi\text{:s cancel}}{=} \frac{-i}{2m}\left[\psi^* \vec{\pi}^2 \psi - \psi(\vec{\pi}^2\psi)^*\right] \\
&= \frac{-i}{2m}\left[\psi^*(\vec{p} - \vec{A})^2\psi - \psi\big((\vec{p} - \vec{A})^2\psi\big)^*\right] \\
&= \frac{-i}{2m}\left[\psi^*(-i\vec{\nabla} - \vec{A})^2\psi - \psi(i\vec{\nabla} - \vec{A})^2\psi^*\right] \\
&= \frac{-i}{2m}\left[\psi^*(-\vec{\nabla}^2 + i\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot i\vec{\nabla} + \vec{A}^2)\psi - \psi(-\vec{\nabla}^2 - i\vec{\nabla}\cdot\vec{A} - \vec{A}\cdot i\vec{\nabla} + \vec{A}^2)\psi^*\right] \\
&= \frac{-i}{2m}\left[\psi^*(-\vec{\nabla}^2 + i(\vec{\nabla}\cdot\vec{A}) + 2i\vec{A}\cdot\vec{\nabla} + \vec{A}^2)\psi - \psi(-\vec{\nabla}^2 - i(\vec{\nabla}\cdot\vec{A}) - 2i\vec{A}\cdot\vec{\nabla} + \vec{A}^2)\psi^*\right] \\
&\overset{\vec{A}^2\text{ cancels}}{=} \frac{-i}{2m}\left[\psi^*(-\vec{\nabla}^2 + 2i\vec{A}\cdot\vec{\nabla})\psi + 2i\psi^*(\vec{\nabla}\cdot\vec{A})\psi - \psi(-\vec{\nabla}^2 - 2i\vec{A}\cdot\vec{\nabla})\psi^*\right].
\end{aligned} \tag{3}$$

Secondly, by (1),

$$\begin{aligned}
\vec{\nabla}\cdot\vec{\jmath} &= \frac{1}{2m}\vec{\nabla}\cdot\left[\psi^*\vec{\pi}\psi+\psi(\vec{\pi}\psi)^*\right]\\
&= \frac{1}{2m}\vec{\nabla}\cdot\left[\psi^*(\vec{p}-\vec{A})\psi+\psi\big((\vec{p}-\vec{A})\psi\big)^*\right]\\
&= \frac{1}{2m}\vec{\nabla}\cdot\left[\psi^*(-i\vec{\nabla}-\vec{A})\psi+\psi(i\vec{\nabla}-\vec{A})\psi^*\right]\\
&= \frac{-i}{2m}\vec{\nabla}\cdot\left[\psi^*(\vec{\nabla}\psi)-i\psi^*\vec{A}\psi-\psi(\vec{\nabla}\psi^*)-i\psi\vec{A}\psi^*\right]\\
&= \frac{-i}{2m}\Big[(\vec{\nabla}\psi^*)\cdot(\vec{\nabla}\psi)+\psi^*(\vec{\nabla}^2\psi)-i(\vec{\nabla}\psi^*)\cdot\vec{A}\psi-i\psi^*(\vec{\nabla}\cdot\vec{A})\psi-i\psi^*\vec{A}\cdot(\vec{\nabla}\psi)\\
&\qquad -(\vec{\nabla}\psi)\cdot(\vec{\nabla}\psi^*)-\psi(\vec{\nabla}^2\psi^*)-i(\vec{\nabla}\psi)\cdot\vec{A}\psi^*-i\psi(\vec{\nabla}\cdot\vec{A})\psi^*-i\psi\vec{A}\cdot(\vec{\nabla}\psi^*)\Big]\\
&\overset{\substack{(\vec{\nabla}\psi^*)\cdot(\vec{\nabla}\psi)\\ \text{cancels}}}{=} \frac{-i}{2m}\left[-\psi^*(-\vec{\nabla}^2+2i\vec{A}\cdot\vec{\nabla})\psi-2i\psi^*(\vec{\nabla}\cdot\vec{A})\psi-\psi(-\vec{\nabla}^2-2i\vec{A}\cdot\vec{\nabla})\psi^*\right].
\end{aligned}\tag{4}$$

Since (3) $= -$(4), we have shown that our definition (1) satisfies the continuity equation (2).

We now want to show that our definition is gauge invariant. Consider a gauge transform $\vec{A}\mapsto\vec{A}+\vec{\nabla}\Lambda$ ($\vec{\jmath}$ independent of the potential ϕ so we don't have to consider those transformations). We have that

$$\vec{A}\mapsto\vec{A}+\vec{\nabla}\Lambda \tag{5}$$
$$\psi\mapsto \mathrm{e}^{i\Lambda}\psi \tag{6}$$
$$\psi^*\mapsto \mathrm{e}^{-i\Lambda}\psi^* \tag{7}$$

and

$$\psi\mathrm{e}^{i\Lambda}=\mathrm{e}^{i\Lambda}\psi \tag{8}$$
$$\vec{A}\mathrm{e}^{i\Lambda}=\mathrm{e}^{i\Lambda}\vec{A} \tag{9}$$
$$\vec{\nabla}\Lambda\mathrm{e}^{i\Lambda}=\mathrm{e}^{i\Lambda}\vec{\nabla}\Lambda \tag{10}$$
$$\vec{p}\mathrm{e}^{i\Lambda}=\mathrm{e}^{i\Lambda}(\vec{p}+\vec{\nabla}\Lambda). \tag{11}$$

Where the last identity comes from using the product and chain rule. It now follows that

$$\begin{aligned}
\vec{\jmath} &= \frac{1}{2m}\left[\psi^*(\vec{p}-\vec{A})\psi-\psi\big((\vec{p}-\vec{A})\psi\big)^*\right]\\
&\overset{(5),\,(6)\text{ and }(7)}{\mapsto} \frac{1}{2m}\left[\mathrm{e}^{-i\Lambda}\psi^*(\vec{p}-\vec{A}-\vec{\nabla}\Lambda)\mathrm{e}^{i\Lambda}\psi-\mathrm{e}^{i\Lambda}\psi\big((\vec{p}-\vec{A}-\vec{\nabla}\Lambda)\mathrm{e}^{i\Lambda}\psi\big)^*\right]\\
&\overset{(9),\,(10)\text{ and }(11)}{=} \frac{1}{2m}\left[\mathrm{e}^{-i\Lambda}\psi^*\mathrm{e}^{i\Lambda}(\vec{p}-\vec{A})\psi-\mathrm{e}^{i\Lambda}\psi\big(\mathrm{e}^{i\Lambda}(\vec{p}-\vec{A})\psi\big)^*\right]\\
&\overset{(8)}{=} \frac{1}{2m}\left[\psi^*(\vec{p}-\vec{A})\psi-\psi\big((\vec{p}-\vec{A})\psi\big)^*\right]\\
&= \vec{\jmath}.
\end{aligned}\tag{12}$$

Hence the probability flux $\vec{\jmath}$ is gauge invariant.

2 Problem 2 ass #4

Two twins (Philippe and Filip) studying the MPPHS programme decide to carry out the following experiment: They set up a light source that emits two photons at a time, back-to-back in the laboratory frame. The density matrix of the system is given by:

$$\rho = \frac{1}{2} \left(|\mathrm{LL}\rangle \langle \mathrm{LL}| + |\mathrm{RR}\rangle \langle \mathrm{RR}| \right)$$

where "L" refers to left-handed circular polarization, and "R" refers to right-handed circular polarization. Thus, $|\mathrm{LR}\rangle$ would refer to a state in which photon number 1 (defined as the photon which is aimed at Philippe) is left-handed, and photon number 2 (the photon aimed at Filip) is right-handed.

The twins (one of whom is of a diabolical bent) decide to play a game with nature: Philippe stays in the lab, while Filip treks to a point half a light-year away. The light source is turned on and emits two photons, one directed toward each student. Philippe soon measures the polarization of his photon; it is left-handed. He quickly makes a note to his brother that he is going to see a left-handed photon, some time after next Midsommar. Midsommar has come and gone, and finally Filip sees his photon, and measures its polarization. He sends a message back to Philippe, who learns in yet another half year what he knew all along: Filip's photon was left-handed.

Philippe then has a sneaky idea. He secretly changes the apparatus, without telling his forlorn brother. Now the density operator is:

$$\frac{1}{2} \left(|\mathrm{LL}\rangle + |\mathrm{RR}\rangle \right) \left(\langle \mathrm{LL}| + \langle \mathrm{RR}| \right)$$

He causes another pair of photons to be emitted with this new apparatus, and repeats the experiment. The result is identical to the first experiment.

(a) For each apparatus, is the ensemble pure or mixed? Was Philippe just lucky in predicting Filip's measurement result, or will he get the right answer every time, for each apparatus? Demonstrate your answer explicitly, in the density matrix formalism.

(b) What is the probability that Filip will observe a left-handed photon, or a right-handed photon, for each apparatus? Is there a problem with causality here? How can Philippe know what Filip is going to see, long before he sees it? Discuss! Feel free to modify the experiment to illustrate any points you wish to make.

2.1 Solution

Calculations for this problem are presented in section 2.2.

Choose the basis $\{|\mathrm{LL}\rangle, |\mathrm{LR}\rangle, |\mathrm{RL}\rangle, |\mathrm{RR}\rangle\}$ for the product space of the two photons (realized as the Krönecker products $|\mathrm{L}\rangle \otimes |\mathrm{L}\rangle \doteq \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $|\mathrm{L}\rangle \otimes |\mathrm{R}\rangle \doteq \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, etc). Then

$$\frac{1}{2} \left(|\mathrm{LL}\rangle \langle \mathrm{LL}| + |\mathrm{RR}\rangle \langle \mathrm{RR}| \right) \doteq \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{13}$$

Call this operator ρ_1. We also have

$$\frac{1}{2} \left(|\mathrm{LL}\rangle + |\mathrm{RR}\rangle \right) \left(\langle \mathrm{LL}| + \langle \mathrm{RR}| \right) \doteq \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}. \tag{14}$$

Which we'll call ρ_2.

The density matrix of an ensemble is a sum of outer products

$$\rho = \sum_i c_i |\psi_i\rangle \langle \psi_i| .$$

It is in a pure state iff it can be written as a single outer product

$$\rho = |\psi\rangle \langle\psi| ,$$

Under the condition that ρ has trace 1, this is equivalent to ρ being a projection operator.

We have

$$\rho_1^2 \neq \rho_1$$
$$\rho_2^2 = \rho_2$$

and thus the first ensemble is mixed while the second ensemble is pure. This is also more or less clear by inspecting (13) and (14) directly.

Philippe will always be able to tell which state Filip measures since

1. for the the first ensemble, with density matrix ρ_1,
   (a) if Phillipe measures L, then he knows the apparatus must have sent out the state $|\mathrm{LL}\rangle$, and thus Filip must measure L
   (b) if Phillipe measures R, then he knows the apparatus must have sent out the state $|\mathrm{RR}\rangle$, and thus Filip must measure R
2. for the the first ensemble, with density matrix ρ_2,
   (a) if Phillipe measures L, then he has "collapsed" the state into $|\mathrm{LL}\rangle$, and thus Filip must measure L
   (b) if Phillipe measures R, then he has "collapsed" the state into $|\mathrm{RR}\rangle$, and thus Filip must measure R.

The probability that Filip will measure L is the expectation value of the operator

$$\mathcal{O}_{\mathrm{F}} = I \otimes \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

which measures 1 if Filip's photon is L and measures 0 if Filip's photon is R. For the first ensamble,

$$P(\text{Filip measures L}) = \langle \mathcal{O}_F \rangle = \operatorname{tr} \rho_1 \mathcal{O}_F = \frac{1}{2}.$$

For the second ensamble,

$$P(\text{Filip measures L}) = \langle \mathcal{O}_F \rangle = \operatorname{tr} \rho_2 \mathcal{O}_F = \frac{1}{2}.$$

I do not think there is a problem with causality because no information can be transmitted by making measurements. Filip cannot tell if Phillipe has measured or not by making measurements on his photon.

The reason Phillipe knows what Filip is going to see long before he sees it is that

1. for the first apparatus, the photons are always the same polarization
2. for the second apparatus, the photons are entangled.

For the second apparatus, one can either view it as Phillip collapsing the state when measuring and that way sending a photon of definite polarization on its way to Filip, or one can view it as Phillipe becoming entagled with the state. When Filip finally measures his photon, he becomes entangled with it and thus becomes entangled with Phillipe. Any outside observer trying to ask Phillipe or Filip which polarization they measured will become entagled with the whole quantum system of brothers and photons. In this framework I think it is a little bit easier to accept that nothing breaks causality.

As a sidenote I found an operator

$$A = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

which can be used to differentiate between the systems, as its expected values are

1. 0 for ensemble 1
2. 1 for ensemble 2.

Notice that it nessecarily is not a "pure" tensor product of two operators.

2.2 Mathematica code

ClearAll["Global`*"]

(*Write down basis elements*)

$$\mathbf{LLket} = \mathbf{KroneckerProduct}\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right]; \mathbf{LLbra} = \mathbf{Transpose[LLket]};$$

$$\mathbf{LRket} = \mathbf{KroneckerProduct}\left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right]; \mathbf{LRbra} = \mathbf{Transpose[LRket]};$$

$$\mathbf{RLket} = \mathbf{KroneckerProduct}\left[\begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right]; \mathbf{RLbra} = \mathbf{Transpose[RLket]};$$

$$\mathbf{RRket} = \mathbf{KroneckerProduct}\left[\begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right]; \mathbf{RRbra} = \mathbf{Transpose[RRket]};$$

(*Write down destiny operators*)

$\boldsymbol{\rho 1} = \frac{1}{2}\mathbf{(LLket.LLbra + RRket.RRbra);}$

$\boldsymbol{\rho 2} = \frac{1}{2}\mathbf{(LLket + RRket).(LLbra + RRbra);}$

$\mathbf{Print}\left[\text{"}\boldsymbol{\rho 1} = \frac{1}{2}\text{"}, \mathbf{MatrixForm}[2\boldsymbol{\rho 1}]\right];$

$\mathbf{Print}\left[\text{"}\boldsymbol{\rho 2} = \frac{1}{2}\text{"}, \mathbf{MatrixForm}[2\boldsymbol{\rho 2}]\right];$

$$\rho 1 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\rho 2 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}$$

(*Check if ρ1 is a mixed state*)

$\rho 1.\rho 1 == \rho 1$

False

(*Check if ρ2 is a mixed state*)

$\rho 2.\rho 2{=}{=}\rho 2$

True

(*Calculate probability that Filip measures L*)

$$\mathbf{OF = KroneckerProduct}\left[\left(\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right), \mathbf{IdentityMatrix[2]}\right];$$

Print[“<OF> = ”, Tr[ρ1.OF], “ for ensemble 1”]

Print[“<OF> = ”, Tr[ρ2.OF], “ for ensemble 2”]

<OF> = $\frac{1}{2}$ for ensemble 1
<OF> = $\frac{1}{2}$ for ensemble 2

(*Define my own operator and calculate its ensemble average*)

A = LLket.RRbra + RRket.LLbra;

MatrixForm[A]

Print[“<A> = ”, Tr[ρ1.A], “ for ensemble 1”]

Print[“<A> = ”, Tr[ρ2.A], “ for ensemble 2”]

$$\left(\begin{array}{cccc} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{array}\right)$$

<A> = 0 for ensemble 1
<A> = 1 for ensemble 2

(*Calculate eigenvectors and eigenvalues of A*)

MatrixForm[Eigensystem[A]]

$$\left(\begin{array}{cccc} -1 & 1 & 0 & 0 \\ \{-1,0,0,1\} & \{-1,0,0,-1\} & \{0,0,1,0\} & \{0,1,0,0\} \end{array}\right)$$

3 Problem 4 ass # 4

Calculate the lifetime of the 2P excited state of the hydrogen atom. What transitions from the 2P state are possible? To calculate the transition rates, you can use the Fermi golden rule,

$$\Gamma = \frac{2\pi}{\hbar} \left|\langle u_f| - \mathbf{d} \cdot \mathbf{1}_\epsilon |u_i\rangle\right|^2 \rho(\omega)\delta(E_i - E_f - \hbar\omega) \tag{15}$$

where ρ is the density of states (you have calculated this already twice before in previous assignments!). Don't forget that photons in different polarization states can be emitted. When there are different decay channels, you need to sum the transition rates (since the rates are essentially probabilities per time unit and probabilities add up). In the final step, then, calculate the lifetime from the total transition rate.

3.1 Solution

The solution is presented in section 3.2.

3.2 Mathematica code

In[1]:=
```
ClearAll["Global`*"]
$Assumptions = (a ∈ Reals && a > 0 && (*Bohr radius*)
    e ∈ Reals && e > 0 && (*elementary charge*)
    me ∈ Reals && me > 0 && (*mass of electron*)
    ϵ0 ∈ Reals && ϵ0 > 0 && (*vacuum permittivity*)
    ℏ ∈ Reals && ℏ > 0 && (*Planck's reducedconstant*)
    c ∈ Reals && c > 0);(*speed of light*)

(*Write down analytical solutions to the hydrogen SE*)
Z = 1;
```

$$\text{R10[r\_]} := 2\, e^{-\frac{r}{a}} \left(\frac{Z}{a}\right)^{3/2}$$

$$\text{R20[r\_]} := \frac{e^{-\frac{r}{2a}} \left(\frac{Z}{a}\right)^{3/2} \left(2 - \frac{r Z}{2}\right)}{2\sqrt{2}}$$

$$\text{R21[r\_]} := \frac{e^{-\frac{r}{2a}}\, r \left(\frac{Z}{a}\right)^{3/2}}{2\sqrt{6}\, a}$$

$$\text{Y00}[\theta\_,\ \varphi\_] := \frac{1}{\sqrt{4\pi}}$$

$$\text{Y10}[\theta\_,\ \varphi\_] := \frac{1}{2}\sqrt{\frac{3}{\pi}}\ \text{Cos}[\theta]$$

$$\text{Y11}[\theta\_,\ \varphi\_] := -\, e^{i\varphi}\sqrt{\frac{3}{8\pi}}\ \text{Sin}[\theta]$$

$$\text{Y1m1}[\theta\_,\ \varphi\_] := e^{-i\varphi}\sqrt{\frac{3}{8\pi}}\ \text{Sin}[\theta]$$

In[11]:=
```
(*Define some factors appearing in the integrand in Fermi's golden rule*)
dipole[r_, θ_, φ_] := -e r (Sin[θ] Cos[φ] + Sin[θ] Sin[φ] + Cos[θ]) (*-d·1_ϵ*)
```

$$\text{jacobian}[r\_,\ \theta\_,\ \varphi\_] := r^2\ \text{Sin}[\theta]\text{(*Spherical coordinates Jacobian*)}$$

$$\rho[\omega\_] := \frac{\omega^2}{c^3\, \pi^2}\text{(*Density of states*)}$$

```
(*Loop through different possible decays and calculate their transition rates*)
uiList = {R21[r] × Y10[θ, φ],
   R21[r] × Y10[θ, φ],
   R21[r] × Y10[θ, φ],
   R21[r] × Y10[θ, φ],
   R21[r] × Y11[θ, φ],
   R21[r] × Y11[θ, φ],
   R21[r] × Y11[θ, φ],
   R21[r] × Y11[θ, φ],
   R21[r] × Y1m1[θ, φ],
   R21[r] × Y1m1[θ, φ],
   R21[r] × Y1m1[θ, φ],
   R21[r] × Y1m1[θ, φ]};
nlmInitialList = {{2, 1, 0},
   {2, 1, 0},
   {2, 1, 0},
   {2, 1, 0},
   {2, 1, 1},
   {2, 1, 1},
   {2, 1, 1},
   {2, 1, 1},
   {2, 1, -1},
   {2, 1, -1},
   {2, 1, -1},
   {2, 1, -1}};
ufList = {R10[r] × Y00[θ, φ],
   R20[r] × Y00[θ, φ],
   R21[r] × Y11[θ, φ],
   R21[r] × Y1m1[θ, φ],
   R10[r] × Y00[θ, φ],
   R20[r] × Y00[θ, φ],
   R21[r] × Y10[θ, φ],
   R21[r] × Y1m1[θ, φ],
   R10[r] × Y00[θ, φ],
   R20[r] × Y00[θ, φ],
   R21[r] × Y10[θ, φ],
   R21[r] × Y11[θ, φ]};
nlmFinalList = {{1, 0, 0},
   {2, 0, 0},
   {2, 1, 1},
   {2, 1, -1},
   {1, 0, 0},
   {2, 0, 0},
```

```
    {2, 1, 0},
    {2, 1, -1},
    {1, 0, 0},
    {2, 0, 0},
    {2, 1, 0},
    {2, 1, 1}};

ΓList = Range[Length[uiList]];(*Initiate*)
For[i = 1, i <= Length[uiList], i++,
 (*Define initial and final wavefunctions*)
 ui[r_, θ_, φ_] = uiList[[i]];
 nlmInitial = nlmInitialList[[i]];
 nInitial = nlmInitial[[1]];
 Ei = -(e^4 me)/(2 (4 π ϵ0)^2 ℏ^2) 1/nInitial^2; (*energy of initial state*)
 uf[r_, θ_, φ_] = ufList[[i]];
 nlmFinal = nlmFinalList[[i]];
 nFinal = nlmFinal[[1]];
 Ef = -(e^4 me)/(2 (4 π ϵ0)^2 ℏ^2) 1/nFinal^2; (*energy of final state*)
 ω = (Ei - Ef) / ℏ ;

 (*Calculate the braket appearing in Fermi's golden rule*)
 integrand[r_, θ_, φ_] := uf[r, θ, φ] × dipole[r, θ, φ] × ui[r, θ, φ];
 braket = Integrate[
   Integrate[
    Integrate[
     integrand[r, θ, φ] × jacobian[r, θ, φ],
     {φ, 0, 2 π}],
    {θ, 0, π}],
   {r, 0, Infinity}];

 (*Calculate and print transition rates*)
 Γ = 1/(4 π ϵ0) ω (2 π)/ℏ Abs[braket]^2 ρ[ω];
 ΓList[[i]] = Γ;
 Print["from |ui>=|", nlmInitial[[1]], nlmInitial[[2]], nlmInitial[[3]],
  "> to |uf>=|", nlmFinal[[1]], nlmFinal[[2]], nlmFinal[[3]], ">, Γ=", FullSimplify[Γ]]

]
```

from |ui>=|210> to |uf>=|100>, $\Gamma = \frac{a^2\, e^{14}\, me^3}{279\,936\, c^3\, \pi^8\, \epsilon 0^7\, \hbar^{10}}$

from |ui>=|210> to |uf>=|200>, Γ=0

from |ui>=|210> to |uf>=|211>, Γ=0

from |ui>=|210> to |uf>=|21-1>, Γ=0

from |ui>=|211> to |uf>=|100>, $\Gamma = \frac{a^2\, e^{14}\, me^3}{279\,936\, c^3\, \pi^8\, \epsilon 0^7\, \hbar^{10}}$

from |ui>=|211> to |uf>=|200>, Γ=0

from |ui>=|211> to |uf>=|210>, Γ=0

from |ui>=|211> to |uf>=|21-1>, Γ=0

from |ui>=|21-1> to |uf>=|100>, $\Gamma = \frac{a^2\, e^{14}\, me^3}{279\,936\, c^3\, \pi^8\, \epsilon 0^7\, \hbar^{10}}$

from |ui>=|21-1> to |uf>=|200>, Γ=0

from |ui>=|21-1> to |uf>=|210>, Γ=0

from |ui>=|21-1> to |uf>=|211>, Γ=0

In[20]:=
```
(*Evaluate expression in SI units*)
(*Half life should be ~1.6 ns*)
a = Quantity["BohrRadius"];
e = Quantity["ElementaryCharge"];
me = Quantity["ElectronMass"];
c = Quantity["SpeedOfLight"];
ϵ0 = Quantity["VacuumPermittivity"];
ℏ = Quantity["hbar"];

Print["Γ = ", UnitConvert[ΓList[[1]]]]
Print["τ = 1/(2Γ) =", UnitConvert[1/(2 ΓList[[1]])]]
```

Γ = 2.9929000×10^{8} per second

τ = $\frac{1}{2\Gamma}$ = $1.67062048 \times 10^{-9}$ s