```
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;
```

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

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

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

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

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

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

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

```
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]) (*−d⃗·1_ϵ*)
```

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

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

```
(*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]];
```

$$Ei = -\frac{e^4\,me}{2\,(4\,\pi\,\epsilon 0)^2\,\hbar^2}\,\frac{1}{nInitial^2};\ \text{(*energy of initial state*)}$$

```
 uf[r_, θ_, φ_] = ufList[[i]];
 nlmFinal = nlmFinalList[[i]];
 nFinal = nlmFinal[[1]];
```

$$Ef = -\frac{e^4\,me}{2\,(4\,\pi\,\epsilon 0)^2\,\hbar^2}\,\frac{1}{nFinal^2};\ \text{(*energy of final state*)}$$

```
 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*)
```

$$\Gamma = \frac{1}{4\,\pi\,\epsilon 0}\,\omega\,\frac{2\,\pi}{\hbar}\,\text{Abs[braket]}^2\,\rho[\omega];$$

```
 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>, $\Gamma = \dfrac{a^2\, e^{14}\, me^3}{279\,936\, c^3\, \pi^8\, \epsilon 0^7\, \hbar^{10}}$

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>, $\Gamma = \dfrac{a^2\, e^{14}\, me^3}{279\,936\, c^3\, \pi^8\, \epsilon 0^7\, \hbar^{10}}$

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>, $\Gamma = \dfrac{a^2\, e^{14}\, me^3}{279\,936\, c^3\, \pi^8\, \epsilon 0^7\, \hbar^{10}}$

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

$\tau = \dfrac{1}{2\,\Gamma} = 1.67062048 \times 10^{-9}$ s