

In[702]:=

```
SetDirectory[NotebookDirectory[]];
(*Defining where the plots must be saved and the list of these paths.*)
overleafDrafpath =
  "/Users/brunogoes/Dropbox/Aplicativos/Overleaf/00Goes-Bruno-PhDThesis/
  Figures/Chap6";
overleafFinalpath =
  "/Users/brunogoes/Dropbox/Aplicativos/Overleaf/01Goes-Bruno-PhDThesis/
  Figures/Chap6/";
overleafNotespath =
  "/Users/brunogoes/Dropbox/Aplicativos/Overleaf/SPI-Magnetic-field/Figures/
  Spontaneous-emission/";
pathsList = {overleafDrafpath, overleafFinalpath, overleafNotespath};
(*PlotStyling*)
fontsize = 24;
alphabetlabel = {"(a)", "(b)", "(c)", "(d)", "(e)", "(f)", "(g)",
  "(h)", "(i)", "(j)", "(k)", "(l)", "(m)", "(n)", "(o)", "(p)", "(q)",
  "(r)", "(s)", "(t)", "(u)", "(v)", "(w)", "(x)", "(y)", "(z)"};
ClearAll[MPLColorMap]
<< "http://pastebin.com/raw/pFsb4ZBS";
MPLColorMap["Inferno"];

Clear[savePlot];
savePlot[nameAndExtension_, plot_, path_ : pathsList] := Do[
  Export[PlotsPath <> nameAndExtension, plot], {PlotsPath, path}]
```

# Chapter 6: SPI subjected to a in-plane magnetic field

Author: Bruno Ortega Goes

Parameters set definitions and loading experimental data/simulations ✓

```
In[10]:= (*All the physical parameter are real*)
$Assumptions =
  {nx2 + ny2 + nz2 == 1 &&
    Ωg > 0 &&
    Ωe > 0 &&
    ΩR > 0 &&
    ΩL > 0 &&
    γ > 0 &&
    Γ > 0};
```

## 2) Exporting experimental data

It is necessary to change the path of the experimental data in your notebook if you want the program to run!

```
In[630]:= PrettyTiming[data150 = Import[
  "/Users/brunogoes/Dropbox/Research-projects/22--SPIMagneticField/
  ExperimentalData/Data/Data_150mT.csv"];
data250 = Import[
  "/Users/brunogoes/Dropbox/Research-projects/22--SPIMagneticField/
  ExperimentalData/Data/Data_250mT.csv"];
data350 = Import[
  "/Users/brunogoes/Dropbox/Research-projects/22--SPIMagneticField/
  ExperimentalData/Data/Data_350mT.csv"];
data450 = Import[
  "/Users/brunogoes/Dropbox/Research-projects/22--SPIMagneticField/
  ExperimentalData/Data/Data_450mT.csv"];]
dataexplist = {data150, data250, data350, data450};
```

0h : 0m : 0s

In[632]:=

```

PrettyTiming[data150dcp = Import[
  "/Users/brunogoes/Dropbox/Research-projects/22--SPIMagneticField/
  ExperimentalData/DataFig2c/Data_150mT_dcp.csv"];
data250dcp = Import[
  "/Users/brunogoes/Dropbox/Research-projects/22--SPIMagneticField/
  ExperimentalData/DataFig2c/Data_250mT_dcp.csv"];
data350dcp = Import[
  "/Users/brunogoes/Dropbox/Research-projects/22--SPIMagneticField/
  ExperimentalData/DataFig2c/Data_350mT_dcp.csv"];
data450dcp = Import[
  "/Users/brunogoes/Dropbox/Research-projects/22--SPIMagneticField/
  ExperimentalData/DataFig2c/Data_450mT_dcp.csv"];
datadcpList = {data150dcp, data250dcp, data350dcp, data450dcp};

```

0h : 0m : 0s

### 3) Parameters Exp.1: Probing the dynamics and coherence of a semiconductor hole spin via acoustic phonon-assisted excitation

In[635]:=

```

Clear[Experimentalγ, ExperimentalΩe, ExperimentalΩg]
τtrion = 450; (*This is constant because it
  depends solely on the cavity used in the experiment*)

Experimentalγ[τtrion_] := 1 / τtrion; (*ps-1*)
ExperimentalΩe[B_] :=  $\left(\frac{0.38 * 58}{658}\right) B (*ps^{-1}*)$ ;
ExperimentalΩg[B_] :=  $\left(\frac{0.38 * 58}{658}\right) B (*ps^{-1}*)$ ;

(*The following experimental physical parameters follow Ref. https://arxiv.org/pdf/2207.05981.pdf*)
PhysicalParameters0 = {Ωe → ExperimentalΩe[0.0] / Experimentalγ[τtrion],
  Ωg → ExperimentalΩg[0.0] / Experimentalγ[τtrion], γ → 1.};
PhysicalParameters30 = {Ωe → ExperimentalΩe[0.03] / Experimentalγ[τtrion],
  Ωg → ExperimentalΩg[0.03] / Experimentalγ[τtrion], γ → 1.};
PhysicalParameters150 = {Ωe → ExperimentalΩe[0.15] / Experimentalγ[τtrion],
  Ωg → ExperimentalΩg[0.15] / Experimentalγ[τtrion], γ → 1.};
PhysicalParameters250 = {Ωe → ExperimentalΩe[0.25] / Experimentalγ[τtrion],
  Ωg → ExperimentalΩg[0.25] / Experimentalγ[τtrion], γ → 1.};
PhysicalParameters350 = {Ωe → ExperimentalΩe[0.35] / Experimentalγ[τtrion],
  Ωg → ExperimentalΩg[0.35] / Experimentalγ[τtrion], γ → 1.};
PhysicalParameters450 = {Ωe → ExperimentalΩe[0.45] / Experimentalγ[τtrion],
  Ωg → ExperimentalΩg[0.45] / Experimentalγ[τtrion], γ → 1.};
PhysicalParameters900 = {Ωe → ExperimentalΩe[0.90] / Experimentalγ[τtrion],
  Ωg → ExperimentalΩg[0.90] / Experimentalγ[τtrion], γ → 1.};

```

```

PhysicalParameters150 =
  {Ω → ExperimentalΩe[0.15] / Experimentalγ[τtrion],
   λ → (ExperimentalΩg[0.15] / Experimentalγ[τtrion]) /
   (ExperimentalΩe[0.15] / Experimentalγ[τtrion]), γ → 1.};

PhysicalParameters250 = {Ω → ExperimentalΩe[0.25] / Experimentalγ[τtrion],
  λ → (ExperimentalΩg[0.25] / Experimentalγ[τtrion]) /
  (ExperimentalΩe[0.25] / Experimentalγ[τtrion]), γ → 1.};

PhysicalParameters350 = {Ω → ExperimentalΩe[0.35] / Experimentalγ[τtrion],
  λ → (ExperimentalΩg[0.35] / Experimentalγ[τtrion]) /
  (ExperimentalΩe[0.35] / Experimentalγ[τtrion]), γ → 1.};

PhysicalParameters450 = {Ω → ExperimentalΩe[0.45] / Experimentalγ[τtrion],
  Ωg → (ExperimentalΩg[0.45] / Experimentalγ[τtrion]) /
  (ExperimentalΩe[0.45] / Experimentalγ[τtrion]), γ → 1.};

Exp1physicalparameterslist =
  {(*PhysicalParameters0,PhysicalParameters30,*)PhysicalParameters150 ,
   PhysicalParameters250, PhysicalParameters350, PhysicalParameters450 };

MagneticFieldDirection = {nx → 1, ny → 0., nz → 0};

texperimentalg2 = 57;
DataTimeRescalingFactorg2 = (2.65 / 0.48);
(*ratio between the maximal points of model and data*)

```

## I. Hilbert space and operators definition ☒

In this section I:

- 1) Define the Hilbert space structure and the operators, it follows the convention  $\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{en}} \otimes \mathcal{H}_{\text{sp}}$  ;
- 2) Obtain the eigenvalues of the density matrix at time t rotated by a general unitary;

Defining the subspaces basis:

For the spin and energy subspaces I have ket0= ketUp = e and ket1= ketDw =g.

In[52]:=

```

ket[0] = ket["upm"] = ket["e"] = Basis[2, 1];
ket[1] = ket["dwm"] = ket["g"] = Basis[2, 2];
(*I added upm and dwm to emphasize that these
  are not the physical spin but the mathematucal ones *)
bra[ket_] := ket* // cf;

```

Defining the basis elements of the spin-energy Hilbert space:  $\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{en}} \otimes \mathcal{H}_{\text{sp}}$ .

In[55]:=

```
Do[
  ket[i, j] = kron[ket[i], ket[j]],
  {i, {"e", "g"}}, {j, {"upm", "dwm"}}
];
```

Defining the operators acting on the total Hilbert space:  $\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{en}} \otimes \mathcal{H}_{\text{sp}}$ .  
I use the same notation as in the thesis.

In[56]:=

```
(*Energy subspace operators*)
(*Remark: Here I added an "E" after  $\sigma$ ,
so that the  $\sigma$ s are the pure Pauli operators always and it
makes it explicit that I'm working on the energy subspace.*)
 $\sigma_E$  = kron[ $\sigma_m$ ,  $\sigma_0$ ];
 $\sigma_{Ex}$  = kron[ $\sigma_x$ ,  $\sigma_0$ ];
 $\sigma_{Ey}$  = kron[ $\sigma_y$ ,  $\sigma_0$ ];
 $\sigma_{Ez}$  = kron[ $\sigma_z$ ,  $\sigma_0$ ];

(*Spin subspace operators*)
s = kron[ $\sigma_0$ ,  $\sigma_m$ ];
sx = kron[ $\sigma_0$ ,  $\sigma_x$ ];
sy = kron[ $\sigma_0$ ,  $\sigma_y$ ];
sz = kron[ $\sigma_0$ ,  $\sigma_z$ ];
```

## II. Rotation operators definition & Coefficients of the wave-function ✓

In this section I:

1) Define the ground and excited state rotation operators

### 1) Definition of the propagators: spontaneous emission, general and simplified ✓

In[201]:=

```
(*I'll assume interaction picture with respect to  $\omega_0$ ,
but I'll carry this factor in all the expressions,
in case we want the general expressions containing it,
it's just a matter of commenting this line*)
 $\omega_0$  = 0;

 $C_e$  =  $\omega_0$  Eye[4] +  $\frac{\Omega}{2}$  sx;

 $C_g$  =  $\frac{\lambda \Omega}{2}$  (nx sx + ny sy + nz sz);
```

In[204]:= **Clear[ $\mathcal{R}g$ ,  $\mathcal{R}e$ ]**

**$\mathcal{R}g[t_] := \text{MatrixExp}[-i t Cg] // \text{cf};$**

**$\mathcal{R}e[t_] := \text{MatrixExp}[-i t Ce] // \text{cf};$**

In[209]:=  **$(\mathcal{R}g[t] \cdot \mathcal{R}g[t]^\dagger // \text{cf}) == \text{Eye}[\text{Length}@\mathcal{R}g[t]]$**

**$(\mathcal{R}e[t]^\dagger \cdot \mathcal{R}e[t] // \text{cf}) == \text{Eye}[\text{Length}@\mathcal{R}e[t]]$**

Out[209]= **True**

Out[210]= **True**

In[211]:=  **$\mathcal{R}e[t] // \text{mf};$**

$$\begin{pmatrix} \cos\left[\frac{t\Omega}{2}\right] & -i \sin\left[\frac{t\Omega}{2}\right] & 0 & 0 \\ -i \sin\left[\frac{t\Omega}{2}\right] & \cos\left[\frac{t\Omega}{2}\right] & 0 & 0 \\ 0 & 0 & \cos\left[\frac{t\Omega}{2}\right] & -i \sin\left[\frac{t\Omega}{2}\right] \\ 0 & 0 & -i \sin\left[\frac{t\Omega}{2}\right] & \cos\left[\frac{t\Omega}{2}\right] \end{pmatrix}$$

In[212]:=  **$\mathcal{R}g[t] // \text{mf};$**

$$\begin{pmatrix} \cos\left[\frac{t\lambda\Omega}{2}\right] - i n_z \sin\left[\frac{t\lambda\Omega}{2}\right] & (-i n_x - n_y) \sin\left[\frac{t\lambda\Omega}{2}\right] & 0 & 0 \\ (-i n_x + n_y) \sin\left[\frac{t\lambda\Omega}{2}\right] & \cos\left[\frac{t\lambda\Omega}{2}\right] + i n_z \sin\left[\frac{t\lambda\Omega}{2}\right] & 0 & 0 \\ 0 & 0 & \cos\left[\frac{t\lambda\Omega}{2}\right] - i n_z \sin\left[\frac{t\lambda\Omega}{2}\right] & (-i n_x - n_y) \sin\left[\frac{t\lambda\Omega}{2}\right] \\ 0 & 0 & (-i n_x + n_y) \sin\left[\frac{t\lambda\Omega}{2}\right] & \cos\left[\frac{t\lambda\Omega}{2}\right] + i n_z \sin\left[\frac{t\lambda\Omega}{2}\right] \end{pmatrix}$$

In[213]:=  **$\text{aveaRaL}[\nu_] := \gamma \text{Exp}[-\gamma t]$**

**$(\text{ket}["e", "upm"] \cdot \mathcal{R}e[t] \cdot \text{ket}["e", \nu]) * (\text{ket}["e", "dwm"] \cdot \mathcal{R}e[t] \cdot \text{ket}["e", \nu])$**

In[214]:=  **$(\text{ket}["e", "dwm"] \cdot \mathcal{R}e[t] \cdot \text{ket}["e", "upm"])$**

**$(\text{ket}["e", "dwm"] \cdot \mathcal{R}e[t] \cdot \text{ket}["e", "dwm"])$**

Out[214]=  $-i \sin\left[\frac{t\Omega}{2}\right]$

Out[215]=  $\cos\left[\frac{t\Omega}{2}\right]$

In[216]:=  **$(\text{ket}["e", "upm"] \cdot \mathcal{R}e[t] \cdot \text{ket}["e", "upm"])$**

**$(\text{ket}["e", "upm"] \cdot \mathcal{R}e[t] \cdot \text{ket}["e", "dwm"])$**

Out[216]=  $\cos\left[\frac{t\Omega}{2}\right]$

Out[217]=  $-i \sin\left[\frac{t\Omega}{2}\right]$

In[218]:=

```

Clear[M0, U0, M, U] (*ne→-i  $\frac{\gamma}{2}$ *)

(*Matrices without drive: Spontaneous emission case*)
M0 = (Ce.σE†.σE - Cg.σE.σE†) + ne σE†.σE // mf; (*ne is just a dummy variable,
this is related to the 'bug' explained in the appendix*)
U0[t_] := MatrixExp[-i t M0] /. ne → -i  $\frac{\gamma}{2}$  // cf;

U0::usage =
  "Takes the evolution time t as an argument. The internal parameters of
  this function that must be defined are: the Larmor frequencies
  Ωe and Ωg, the direction of the magnetic field in the ground
  state (nx,ny,nz), the decay rate γ (usually taken to be 1).";

(*Matrices with drive*)
M = (Ce.σE†.σE - Cg.σE.σE†) +  $\left(\frac{\Omega L}{2} s.s^\dagger + \frac{\Omega R}{2} s^\dagger.s\right).σE_y$  + ne σE†.σE // mf;
U[t_] := MatrixExp[-i t M] /. ne →  $\left(-i \frac{\gamma}{2}\right)$ ;

U::usage =
  "Takes the evolution time t as an argument. The internal parameters of
  this function that must be defined are: the Larmor frequencies
  Ωe and Ωg, the direction of the magnetic field in the ground
  state (nx,ny,nz), the decay rate γ (usually taken to be 1) and
  the drive amplitudes ΩL and ΩR. For ΩL=ΩR=0, i.e. in the absence
  of a drive, we obtain U0, the spontaneous emission case.";

(*Matrices with drive neglecting Overhauser*)
Mmod = M /. λ → 1 /. ΩR → ΩH /. ΩL → ΩH /. nx → 1 /. ny → 0 /. nz → 0 // cf // mf;
Umod[s_] := MatrixExp[-i s Mmod] /. ne → -i  $\frac{\gamma}{2}$ ;

```

$$\begin{pmatrix}
 ne \frac{\Omega}{2} & 0 & 0 \\
 \frac{\Omega}{2} ne & 0 & 0 \\
 0 & 0 & -\frac{1}{2} nz \lambda \Omega & -\frac{1}{2} (nx - i ny) \lambda \Omega \\
 0 & 0 & -\frac{1}{2} (nx + i ny) \lambda \Omega & \frac{nz \lambda \Omega}{2}
 \end{pmatrix}$$

$$\begin{pmatrix}
 ne \frac{\Omega}{2} & -\frac{i \Omega R}{2} & 0 \\
 \frac{\Omega}{2} ne & 0 & -\frac{i \Omega L}{2} \\
 \frac{i \Omega R}{2} & 0 & -\frac{1}{2} nz \lambda \Omega & -\frac{1}{2} (nx - i ny) \lambda \Omega \\
 0 & \frac{i \Omega L}{2} & -\frac{1}{2} (nx + i ny) \lambda \Omega & \frac{nz \lambda \Omega}{2}
 \end{pmatrix}$$

$$\begin{pmatrix}
 ne \frac{\Omega}{2} & -\frac{i \Omega H}{2} & 0 \\
 \frac{\Omega}{2} ne & 0 & -\frac{i \Omega H}{2} \\
 \frac{i \Omega H}{2} & 0 & 0 & -\frac{\Omega}{2} \\
 0 & \frac{i \Omega H}{2} & -\frac{\Omega}{2} & 0
 \end{pmatrix}$$

## 2) Coefficients for spontaneous emission

In[79]:=

```
Clear[f0SE];
f0SE[finalenergy_, finalspin_, initialenergy_, initialspin_, t_] :=
  ket[finalenergy, finalspin].U0[t].ket[initialenergy, initialspin]
f0SE::usage =
  "The order of the arguments is: the system final state: energy and spin,
  the system initial state: energy and spin, and the time variable t.
  The internal parameters of this function that must be defined are:
  the Larmor frequencies  $\Omega_e$  and  $\Omega_g$ , the direction of the magnetic
  field in the ground state (nx,ny,nz), the decay rate  $\gamma$  (by default
  1) and the drive amplitudes  $\Omega_L$  and  $\Omega_R$ . For  $\Omega_L=\Omega_R=0$ , i.e. in the
  absence of a drive, we obtain  $U_0$ , the spontaneous emission case.";
```

In[82]:=

```
Clear[f1RSE];
f1RSE[finalenergy_, finalspin_, initialenergy_, initialspin_, t_, t1_,
   $\gamma_:$  1] :=  $\sqrt{\gamma}$  (ket[finalenergy, finalspin].U0[t-t1].ket["g", "upm"])  $\times$ 
  (ket["e", "upm"].U0[t1].ket[initialenergy, initialspin])
f1RSE::usage = "The order of the arguments is: the system final state:
  energy and spin, the system initial state: energy and spin, the
  time variable t, and the time of photon emission event t1. The
  internal parameters of this function that must be defined are:
  the Larmor frequencies  $\Omega_e$  and  $\Omega_g$ , the direction of the magnetic
  field in the ground state (nx,ny,nz), the decay rate  $\gamma$  (default
  1) and the drive amplitudes  $\Omega_L$  and  $\Omega_R$ . For  $\Omega_L=\Omega_R=0$ , i.e. in the
  absence of a drive, we obtain  $U_0$ , the spontaneous emission case.";
```

In[85]:=

```
Clear[f1LSE];
f1LSE[finalenergy_, finalspin_, initialenergy_, initialspin_, t_, t1_,
   $\gamma_:$  1] :=  $\sqrt{\gamma}$  (ket[finalenergy, finalspin].U0[t-t1].ket["g", "dwm"])  $\times$ 
  (ket["e", "dwm"].U0[t1].ket[initialenergy, initialspin])
f1LSE::usage = "The order of the arguments is: the system final state:
  energy and spin, the system initial state: energy and spin, the
  time variable t, and the time of photon emission event t1. The
  internal parameters of this function that must be defined are: the
  Larmor frequencies  $\Omega_e$  and  $\Omega_g$ , the direction of the magnetic field
  in the ground state (nx,ny,nz), the decay rate  $\gamma$  (usually taken to
  be 1) and the drive amplitudes  $\Omega_L$  and  $\Omega_R$ . For  $\Omega_L=\Omega_R=0$ , i.e. in the
  absence of a drive, we obtain  $U_0$ , the spontaneous emission case.";
```



In[ ]:= (\*Spontaneous emission case coefficients\*)

TextGrid[

{{"Intial Spin", "f0e↑", "f0e↓", "f1Rg↑", "f1Rg↓", "f1Lg↑", "f1Rg↓"},

{"↑",

f0SE["e", "upm", "e", "upm", t],

f0SE["e", "dwm", "e", "upm", t],

f1RSE["g", "upm", "e", "upm", t, t1],

f1RSE["g", "dwm", "e", "upm", t, t1],

f1LSE["g", "upm", "e", "upm", t, t1],

f1LSE["g", "dwm", "e", "upm", t, t1]}},

{"↓",

f0SE["e", "upm", "e", "dwm", t],

f0SE["e", "dwm", "e", "dwm", t],

f1RSE["g", "upm", "e", "dwm", t, t1],

f1RSE["g", "dwm", "e", "dwm", t, t1],

f1LSE["g", "upm", "e", "dwm", t, t1],

f1LSE["g", "dwm", "e", "dwm", t, t1]}},

Frame → All]

Out[ ]:=

Intial Spin	f0e↑	f0e↓	f1Rg↑	f1Rg↓	f1Lg↑	f1Rg↓
↑	$e^{-\frac{t\gamma}{2}} \cos\left[\frac{t\Omega}{2}\right]$	$-i e^{-\frac{t\gamma}{2}} \sin\left[\frac{t\Omega}{2}\right]$	$e^{-\frac{t\gamma}{2}} \cos\left[\frac{t\Omega}{2}\right] \left( \cos\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] + i n z \sin\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] \right)$	$i e^{-\frac{t\gamma}{2}} \cos\left[\frac{t\Omega}{2}\right] \left( (n x + i n y) \cos\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] + \sin\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] \right)$	$-i e^{-\frac{t\gamma}{2}} \sin\left[\frac{t\Omega}{2}\right] \left( (i n x + n y) \cos\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] + \sin\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] \right)$	$-i e^{-\frac{t\gamma}{2}} \sin\left[\frac{t\Omega}{2}\right] \left( \cos\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] - i n z \sin\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] \right)$
↓	$-i e^{-\frac{t\gamma}{2}} \sin\left[\frac{t\Omega}{2}\right]$	$e^{-\frac{t\gamma}{2}} \cos\left[\frac{t\Omega}{2}\right]$	$-i e^{-\frac{t\gamma}{2}} \sin\left[\frac{t\Omega}{2}\right] \left( \cos\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] + i n z \sin\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] \right)$	$e^{-\frac{t\gamma}{2}} \sin\left[\frac{t\Omega}{2}\right] \left( (n x + i n y) \cos\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] + \sin\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] \right)$	$e^{-\frac{t\gamma}{2}} \cos\left[\frac{t\Omega}{2}\right] \left( (i n x + n y) \cos\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] + \sin\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] \right)$	$e^{-\frac{t\gamma}{2}} \cos\left[\frac{t\Omega}{2}\right] \left( \cos\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] - i n z \sin\left[\frac{1}{2}(t-t_1)\lambda\Omega\right] \right)$

Computing the probabilities for the spontaneous emission: Assuming the spin is initially ↑

In[227]:=

```

Clear[P0SE, P1RSE, P1LSE];
Module[{ampR, ampL, initialspin},
  initialspin = "upm";
  PrettyTiming@Do[
    (*Amplitude of no-photon emission squared*)
    P0SE[ef, sf, "e", initialspin, t] =
      f0SE[ef, sf, "e", initialspin, t] × f0SE[ef, sf, "e", initialspin, t]*;

    (*Amplitude of R-photon emission squared and integrate over all t1*)
    ampR = f1RSE[ef, sf, "e", initialspin, t, t1] ×
      f1RSE[ef, sf, "e", initialspin, t, t1]* // cf;
    P1RSE[ef, sf, "e", initialspin, t] = Integrate[ampR, {t1, 0, t}];

    (*Amplitude of L-photon emission squared and integrate over all t1*)
    ampL = f1LSE[ef, sf, "e", initialspin, t, t1] ×
      f1LSE[ef, sf, "e", initialspin, t, t1]* // cf;
    P1LSE[ef, sf, "e", "upm", t] = Integrate[ampL, {t1, 0, t}],

    {ef, {"e", "g"}}, {sf, {"upm", "dwm"}}

  ]
]

```

0h : 2m : 16s

**Sanity check:** Is the wave-function properly normalized?

```

Sum[P0SE[ef, sf, "e", "upm", t] + P1RSE[ef, sf, "e", "upm", t] +
  P1LSE[ef, sf, "e", "upm", t], {ef, {"e", "g"}}, {sf, {"upm", "dwm"}}] // cf

```

Out[ ]= 1

**Yes!**

### 3) Model validation

In[800]:=

```

Clear[DCP];
texperimental = 5.56; (*Used to keep γ=1*)
(*Degree of circular polarization*)
DCP = 
$$\frac{(IRUpSE - ILUpSE)}{(IRUpSE + ILUpSE)}$$
 // cf;

Module[{timescaling, dataset1, dataset2, physicalparameters, epilog},
  timescaling = 5.56 / 2.5 (*Used to keep γ=1*);
  dataset1 = dataexp1list;
  dataset2 = datadcpllist;
  epilog = {"B=150mT", "B=250mT", "B=350mT", "B=450mT"};

```

```

physicalparameters = Exp1physicalparameterslist;
modelValidation = Grid[{
  (*First row*)
  Table[
    Show[
      ListPlot[{
        Table[{dataset1[[k]][i, 1] * timescaling, dataset1[[k]][i, 2]},
          {i, 1, Length@dataset1[[k]]}], Table[{dataset1[[k]][i, 1] * timescaling,
            dataset1[[k]][i, 3]}, {i, 1, Length@dataset1[[k]]}],
        Table[{dataset1[[k]][i, 1] * timescaling, dataset1[[k]][i, 4]},
          {i, 1, Length@dataset1[[k]]}],
        PlotRange → {All, {0, 1}},
        PlotLegends → If[k == 1, legend[{"IR", "IL", "IR+IL"}, {0.8, 0.7}], None],
        FrameLabel → {"γt", "Intensity (arb. unities)"},
        Epilog →
          Inset[Framed[Style[epilog[[k]], Background → LightYellow], {1.5, 0.8}]],

        Plot[{IRUpSE /. physicalparameters[[k]],
          ILUpSE /. physicalparameters[[k]],
          IRUpSE + ILUpSE /. physicalparameters[[k]]},
          {t, 0, texperimental},

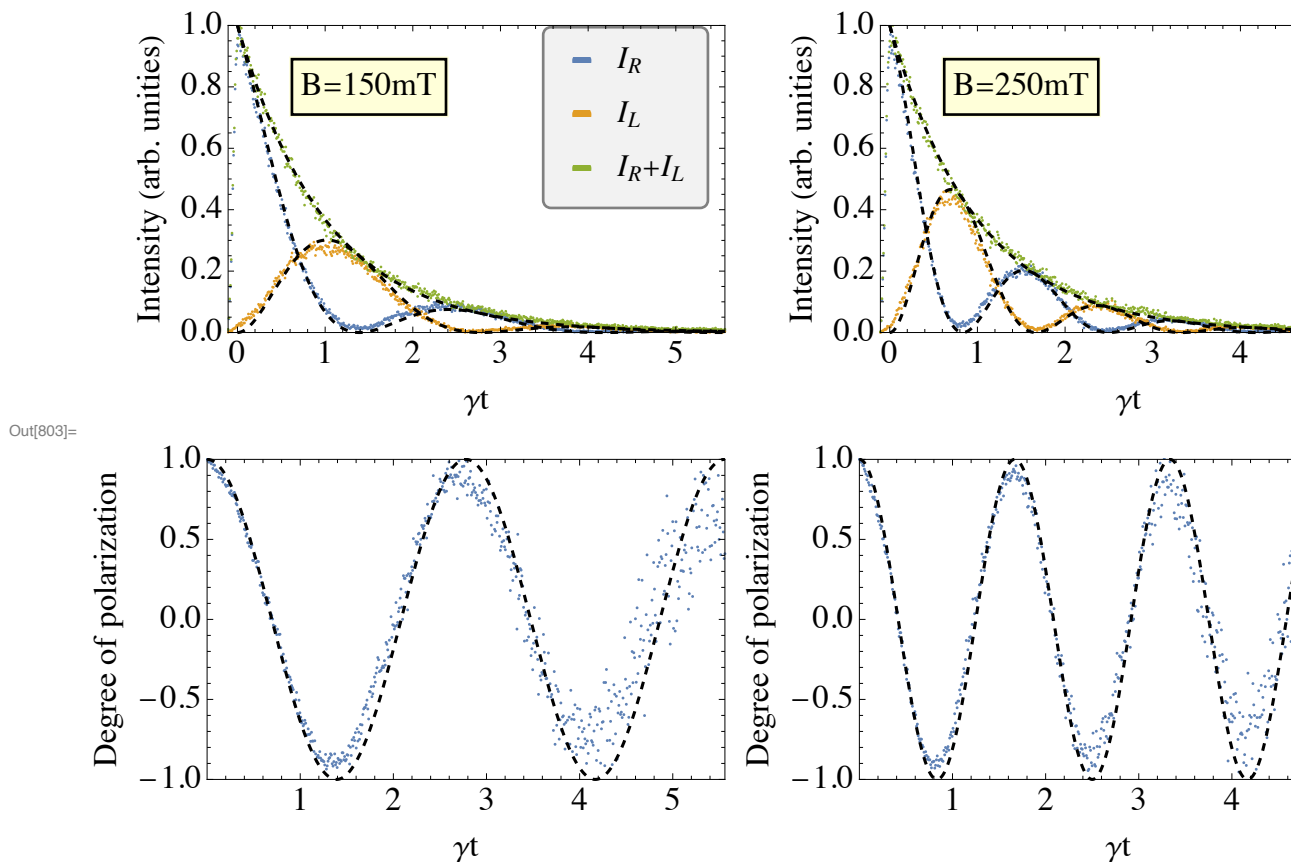
          PlotStyle → {{Black, Dashed}, {Black, Dashed}, {Black, Dashed}},
          PlotRange → {All, {0, 1}},
          PlotLegends → legend[{"IR", "IL", "IR+IL"}, {0.8, 0.7}],
          FrameLabel → {"γt", "Intensity (arb. unities)"},
          Epilog → Inset[Framed[Style[k], Background → LightYellow], {1.5, 0.8}]]
      ],
      {k, 1, Length@dataset1}],

  (*Second row*)
  Table[
    Show[
      ListPlot[
        Table[{dataset2[[k]][i, 1] * (5.56 / 2.5),
          dataset2[[k]][i, 2]}, {i, 1, Length@dataset2[[k]]}],
        PlotRange → {All, {-1, 1}},
        FrameLabel → {"γt", "Degree of polarization"}],

        Plot[DCP /. physicalparameters[[k]], {t, 0, texperimental},
          PlotStyle → {{Black, Dashed}},
          PlotRange → {All, {-1, 1}},
          FrameLabel → {"γt", "Degree of polarization"}]],
      {k, 1, Length@dataset2}
    ]
  }]]
]

```

```
savePlot["modelValidation-ExperimentalDatavsModel.pdf", modelValidation]
```



### III. Fidelity of the spin at the moment of re-excitation ✓

#### 1) Spin state at time t: Analytical calculations ✓

Ideal protocol parameters:

```
In[661]:= idealprotocolparamaters = {γ → 1, nx → 1, ny → 0, nz → 0, λ → 1};
idealalignementparamaters = {γ → 1, nx → 1, ny → 0, nz → 0}; (*λ can change*)
```

```
In[*]:= << overlapsforSpinState.mx
```

In this section I:

- 1) Perform the integrals to obtain the matrix elements of the spin density matrix analytically;
- 2) Obtain the eigenvalues of the density matrix at time t rotated by a general unitary;

Mathematica has some problem with understanding that some parameters are real, so when we conjugate something it considers everything as a complex number. That's why I write all the expressions explicitly and use the cf command (from Melt!) to

FullSimplify considering the parameters real. If I don't do this, Mathematica simply doesn't perform the necessary integrals.

Below I compute all the overlaps for all times, that's to say, I'm not simplifying to the long time limit, so all the expressions below DO HAVE the excited state component.

## a) Computing the overlaps

In[240]:=

```

PrettyTiming[
Module[{FirstTerm, SecondTerm, ThirdTerm,
  Product1, Product2, FirstIntegral, SecondIntegral},

FirstTerm = Exp[-γ t] (ket["e", "upm"]*.Re[t].ket["e", "upm"])* ×
ket["e", "upm"]*.Re[t].ket["e", "upm"] // cf;
(*✓*)

SecondTerm = (ket["g", "upm"]*.Rg[t - u].ket["g", "upm"])* ×
ket["g", "upm"]*.Rg[t - u].ket["g", "upm"] // cf;
(*✓*)

Product1 = f0SE["e", "upm", "e", "upm", u]* ×
f0SE["e", "upm", "e", "upm", u] // cf;
(*✓*)

ThirdTerm = (ket["g", "upm"]*.Rg[t - u].ket["g", "dwm"])* ×
ket["g", "upm"]*.Rg[t - u].ket["g", "dwm"] // cf;
(*✓*)

Product2 = f0SE["e", "dwm", "e", "upm", u]* ×
f0SE["e", "dwm", "e", "upm", u] // cf;
(*✓*)

PrettyTiming[
FirstIntegral = Integrate[SecondTerm Product1 // cf, {u, 0, t}]];
PrettyTiming[SecondIntegral =
Integrate[ThirdTerm Product2 // cf, {u, 0, t}]];

oUpUp = FirstTerm + γ (FirstIntegral + SecondIntegral) /.
(n x2 + n y2) → 1 - n z2 // cf(*✓*);
oUpUpg = γ (FirstIntegral + SecondIntegral) /. (n x2 + n y2) → 1 - n z2 // cf(*✓*);
]
]

```

0h : 0m : 26s

0h : 0m : 39s

0h : 6m : 12s

In[241]:= oUpUp

$$\text{Out[241]} = \frac{1}{4} \times \left( 2 + \frac{e^{i t \lambda \Omega} (-1 + n z^2) \gamma (-i \gamma + \lambda \Omega)}{(i \gamma + \Omega - \lambda \Omega) (\gamma + i (1 + \lambda) \Omega)} + \frac{2 n z^2 \gamma^2}{\gamma^2 + \Omega^2} - \right. \\ \left. \frac{e^{-i t \lambda \Omega} (-1 + n z^2) \gamma (\gamma - i \lambda \Omega)}{\gamma^2 - 2 i \gamma \lambda \Omega + \Omega^2 - \lambda^2 \Omega^2} + \frac{e^{-t (\gamma - i \Omega)} \gamma (-\gamma^2 + 2 i \gamma \Omega + \Omega^2 - n z^2 \lambda^2 \Omega^2)}{(\gamma - i \Omega) (\gamma^2 - 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2)} - \right. \\ \left. \frac{e^{-t (\gamma + i \Omega)} \gamma (\gamma^2 + 2 i \gamma \Omega + (-1 + n z^2 \lambda^2) \Omega^2)}{(\gamma + i \Omega) (\gamma^2 + 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2)} + 2 e^{-t \gamma} \cos[t \Omega] \right)$$

In[242]:= oUpUpg

$$\text{Out[242]} = \frac{1}{8} \times \left( 4 - 4 e^{-t \gamma} + \frac{2 e^{i t \lambda \Omega} (-1 + n z^2) \gamma (-i \gamma + \lambda \Omega)}{(i \gamma + \Omega - \lambda \Omega) (\gamma + i (1 + \lambda) \Omega)} + \frac{4 n z^2 \gamma^2}{\gamma^2 + \Omega^2} - \right. \\ \left. \frac{2 e^{-i t \lambda \Omega} (-1 + n z^2) \gamma (\gamma - i \lambda \Omega)}{\gamma^2 - 2 i \gamma \lambda \Omega - (-1 + \lambda^2) \Omega^2} - \frac{2 e^{-t (\gamma - i \Omega)} \gamma (\gamma^2 - 2 i \gamma \Omega + (-1 + n z^2 \lambda^2) \Omega^2)}{(\gamma - i \Omega) (\gamma^2 - 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2)} - \right. \\ \left. \frac{2 e^{-t (\gamma + i \Omega)} \gamma (\gamma^2 + 2 i \gamma \Omega + (-1 + n z^2 \lambda^2) \Omega^2)}{(\gamma + i \Omega) (\gamma^2 + 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2)} \right)$$

In[243]:=

```

PrettyTiming[
Module[{FirstTerm, SecondTerm, ThirdTerm,
  Product1, Product2, FirstIntegral, SecondIntegral},

FirstTerm = Exp[-γ t] (ket["e", "dwm"]*.Rg[t].ket["e", "upm"])*×
  ket["e", "dwm"]*.Rg[t].ket["e", "upm"] // cf;
(*✓*)

SecondTerm = (ket["g", "dwm"]*.Rg[t - u].ket["g", "upm"])*×
  ket["g", "dwm"]*.Rg[t - u].ket["g", "upm"] // cf;
(*✓*)

Product1 = f0SE["e", "upm", "e", "upm", u]*×
  f0SE["e", "upm", "e", "upm", u] // cf;
(*✓*)

ThirdTerm = (ket["g", "dwm"]*.Rg[t - u].ket["g", "dwm"])*×
  ket["g", "dwm"]*.Rg[t - u].ket["g", "dwm"] // cf;
(*✓*)

Product2 = f0SE["e", "dwm", "e", "upm", u]*×
  f0SE["e", "dwm", "e", "upm", u] // cf;
(*✓*)

FirstIntegral = Integrate[(SecondTerm Product1) // cf, {u, 0, t}];
SecondIntegral = Integrate[(ThirdTerm Product2) // cf, {u, 0, t}];

oDwDw = FirstTerm + γ (FirstIntegral + SecondIntegral) /.
  (nx² + ny²) → 1 - nz² // cf(*✓*);

oDwDwg = γ (FirstIntegral + SecondIntegral) /. (nx² + ny²) → 1 - nz² // cf(*✓*);
]
]

```

0h : 7m : 5s

In[244]:= oDwDw

$$\begin{aligned}
\text{Out[244]} = & \frac{1}{8} \times \left( 4 - \frac{4 n z^2 \gamma^2}{\gamma^2 + \Omega^2} - 4 e^{-t \gamma} \cos[t \Omega] + \right. \\
& \left( 4 e^{-t \gamma} \gamma \left( \gamma \left( \gamma^4 + \gamma^2 \left( 2 + (1 + n z^2) \lambda^2 \right) \Omega^2 + (1 + \lambda^2 + n z^2 \lambda^2 (-3 + \lambda^2)) \Omega^4 \right) \cos[t \Omega] - \right. \right. \\
& \left. \Omega \left( \gamma^4 + \gamma^2 \left( 2 + (-1 + 3 n z^2) \lambda^2 \right) \Omega^2 + (-1 + \lambda^2) \times (-1 + n z^2 \lambda^2) \Omega^4 \right) \sin[t \Omega] + \right. \\
& \left. e^{t \gamma} (-1 + n z^2) \left( \gamma^2 + \Omega^2 \right) \right. \\
& \left. \left( \gamma \left( \gamma^2 + (1 + \lambda^2) \Omega^2 \right) \cos[t \lambda \Omega] + \lambda \Omega \left( \gamma^2 + (-1 + \lambda^2) \Omega^2 \right) \sin[t \lambda \Omega] \right) \right) \right) / \\
& \left( \left( \gamma^2 + \Omega^2 \right) \left( \gamma^2 + (-1 + \lambda)^2 \Omega^2 \right) \left( \gamma^2 + (1 + \lambda)^2 \Omega^2 \right) \right) \Bigg)
\end{aligned}$$

In[245]:= oDwDwg

$$\text{Out[245]} = \frac{1}{4} \times \left( 2 - 2 e^{-t\gamma} - \frac{2 n z^2 \gamma^2}{\gamma^2 + \Omega^2} + \frac{e^{-i t \lambda \Omega} (-1 + n z^2) \gamma (\gamma - i \lambda \Omega)}{\gamma^2 - 2 i \gamma \lambda \Omega - (-1 + \lambda^2) \Omega^2} + \frac{i e^{i t \lambda \Omega} (-1 + n z^2) \gamma (-i \gamma + \lambda \Omega)}{\gamma^2 + 2 i \gamma \lambda \Omega - (-1 + \lambda^2) \Omega^2} + \frac{e^{-t(\gamma - i \Omega)} \gamma (\gamma^2 - 2 i \gamma \Omega + (-1 + n z^2 \lambda^2) \Omega^2)}{(\gamma - i \Omega) (\gamma^2 - 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2)} + \frac{e^{-t(\gamma + i \Omega)} \gamma (\gamma^2 + 2 i \gamma \Omega + (-1 + n z^2 \lambda^2) \Omega^2)}{(\gamma + i \Omega) (\gamma^2 + 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2)} \right)$$

In[246]:=

PrettyTiming[

```
Module[{FirstTerm, SecondTerm, ThirdTerm,
  Product1, Product2, FirstIntegral, SecondIntegral},

FirstTerm = Exp[-γ t] (ket["e", "dwm"]*.Re[t].ket["e", "upm"])*×
ket["e", "upm"]*.Re[t].ket["e", "upm"] // cf;
(*✓*)

SecondTerm = (ket["g", "dwm"]*.Rg[t - u].ket["g", "upm"])*×
ket["g", "upm"]*.Rg[t - u].ket["g", "upm"] // cf;
Product1 = f0SE["e", "upm", "e", "upm", u]*×
f0SE["e", "upm", "e", "upm", u] // cf;
(*✓*)

ThirdTerm = (ket["g", "dwm"]*.Rg[t - u].ket["g", "dwm"])*×
ket["g", "upm"]*.Rg[t - u].ket["g", "dwm"] // cf;
(*✓-There was a correction here! The not conjugated
part was swaped the Up and Dw*)
Product2 = f0SE["e", "dwm", "e", "upm", u]*×
f0SE["e", "dwm", "e", "upm", u] // cf;
(*✓*)

FirstIntegral = Integrate[(SecondTerm Product1) // cf, {u, 0, t}];
SecondIntegral = Integrate[(ThirdTerm Product2) // cf, {u, 0, t}];

oDwUp = FirstTerm + γ (FirstIntegral + SecondIntegral) // cf;

oDwUpg = γ (FirstIntegral + SecondIntegral) // cf;

]
```

0h : 10m : 43s



In[247]:= **oDwUp**Out[247]=  $\frac{1}{4} \times$ 

$$\begin{aligned} & \left( 2 \, i \, e^{-t \gamma} \operatorname{Sin}[t \, \Omega] - \left( 2 \, (n_x - i \, n_y) \, \gamma \left( n_z \, \gamma \left( -\gamma^4 - 2 \, \gamma^2 \, (1 + \lambda^2) \, \Omega^2 - (-1 + \lambda^2)^2 \, \Omega^4 \right) + (\gamma^2 + \Omega^2) \right. \right. \right. \\ & \quad \left. \left. \left( i \, \lambda \, \Omega \left( \gamma^2 + (-1 + \lambda^2) \, \Omega^2 \right) + n_z \, \gamma \left( \gamma^2 + (1 + \lambda^2) \, \Omega^2 \right) \right) \operatorname{Cos}[t \, \lambda \, \Omega] + \right. \right. \\ & \quad e^{-t \gamma} \, \lambda \, \Omega \left( (-i \, \gamma^4 + n_z \, \gamma^3 \, \lambda \, \Omega - i \, \gamma^2 \, \lambda^2 \, \Omega^2 + n_z \, \gamma \, \lambda \, (-3 + \lambda^2) \, \Omega^3 - i \, (-1 + \lambda^2) \, \Omega^4) \right. \\ & \quad \left. \left. \operatorname{Cos}[t \, \Omega] + \Omega \left( 2 \, i \, \gamma^3 - 3 \, n_z \, \gamma^2 \, \lambda \, \Omega + 2 \, i \, \gamma \, \Omega^2 - n_z \, \lambda \, (-1 + \lambda^2) \, \Omega^3 \right) \operatorname{Sin}[t \, \Omega] \right) + \right. \\ & \quad \left. \left. (\gamma^2 + \Omega^2) \left( -i \, \gamma^3 + n_z \, \gamma^2 \, \lambda \, \Omega - i \, \gamma \, (1 + \lambda^2) \, \Omega^2 + n_z \, \lambda \, (-1 + \lambda^2) \, \Omega^3 \right) \operatorname{Sin}[t \, \lambda \, \Omega] \right) \right) \right) / \\ & \quad \left( \gamma^6 + \gamma^4 \left( 3 + 2 \, \lambda^2 \right) \, \Omega^2 + \gamma^2 \left( 3 + \lambda^4 \right) \, \Omega^4 + (-1 + \lambda^2)^2 \, \Omega^6 \right) \end{aligned}$$

In[248]:= **oDwUpg**

$$\begin{aligned} \text{Out[248]} = & - \left( e^{-2 \, t \, \gamma + i \, t \, (-1 + \lambda) \, \Omega} \, (n_x - i \, n_y) \, \gamma \right. \\ & \left( e^{2 \, t \, \gamma + i \, t \, \Omega} \, (-1 + n_z) \, (\gamma - i \, \Omega) \, (\gamma + i \, \Omega) \, (\gamma - i \, (-1 + \lambda) \, \Omega) \, (\gamma + i \, \lambda \, \Omega) \, (\gamma - i \, (1 + \lambda) \, \Omega) + \right. \\ & e^{t \, (2 \, \gamma + i \, (1 - 2 \, \lambda) \, \Omega)} \, (1 + n_z) \, (\gamma - i \, \Omega) \, (\gamma + i \, \Omega) \, (\gamma + i \, (-1 + \lambda) \, \Omega) \, (\gamma - i \, \lambda \, \Omega) \\ & \quad \left. (\gamma + i \, (1 + \lambda) \, \Omega) - 2 \, e^{t \, (2 \, \gamma - i \, (-1 + \lambda) \, \Omega)} \, n_z \, \gamma \left( \gamma^2 + (-1 + \lambda)^2 \, \Omega^2 \right) \left( \gamma^2 + (1 + \lambda)^2 \, \Omega^2 \right) + \right. \\ & e^{t \, (\gamma - i \, \lambda \, \Omega)} \, \lambda \, (\gamma - i \, \Omega) \, \Omega \, (-i \, \gamma + \Omega + n_z \, \lambda \, \Omega) \left( \gamma^2 - 2 \, i \, \gamma \, \Omega + (-1 + \lambda^2) \, \Omega^2 \right) + \\ & \quad \left. e^{t \, (\gamma - i \, (-2 + \lambda) \, \Omega)} \, \lambda \, (\gamma + i \, \Omega) \, \Omega \, (-i \, \gamma + (-1 + n_z \, \lambda) \, \Omega) \left( \gamma^2 + 2 \, i \, \gamma \, \Omega + (-1 + \lambda^2) \, \Omega^2 \right) \right) \right) / \\ & \left( 4 \left( \gamma^2 + \Omega^2 \right) \left( \gamma^4 + 2 \, \gamma^2 \left( 1 + \lambda^2 \right) \, \Omega^2 + (-1 + \lambda^2)^2 \, \Omega^4 \right) \right) \end{aligned}$$

In[249]:= **oUpDw = Conjugate[oDwUp]**

$$\begin{aligned} \text{Out[249]} = & \frac{1}{4} \operatorname{Conjugate} \left[ \right. \\ & 2 \, i \, e^{-t \gamma} \operatorname{Sin}[t \, \Omega] - \left( 2 \, (n_x - i \, n_y) \, \gamma \left( n_z \, \gamma \left( -\gamma^4 - 2 \, \gamma^2 \, (1 + \lambda^2) \, \Omega^2 - (-1 + \lambda^2)^2 \, \Omega^4 \right) + (\gamma^2 + \Omega^2) \right. \right. \\ & \quad \left. \left( i \, \lambda \, \Omega \left( \gamma^2 + (-1 + \lambda^2) \, \Omega^2 \right) + n_z \, \gamma \left( \gamma^2 + (1 + \lambda^2) \, \Omega^2 \right) \right) \operatorname{Cos}[t \, \lambda \, \Omega] + \right. \\ & \quad e^{-t \gamma} \, \lambda \, \Omega \left( (-i \, \gamma^4 + n_z \, \gamma^3 \, \lambda \, \Omega - i \, \gamma^2 \, \lambda^2 \, \Omega^2 + n_z \, \gamma \, \lambda \, (-3 + \lambda^2) \, \Omega^3 - i \, (-1 + \lambda^2) \, \Omega^4) \right. \\ & \quad \left. \left. \operatorname{Cos}[t \, \Omega] + \Omega \left( 2 \, i \, \gamma^3 - 3 \, n_z \, \gamma^2 \, \lambda \, \Omega + 2 \, i \, \gamma \, \Omega^2 - n_z \, \lambda \, (-1 + \lambda^2) \, \Omega^3 \right) \operatorname{Sin}[t \, \Omega] \right) + \right. \\ & \quad \left. \left. (\gamma^2 + \Omega^2) \left( -i \, \gamma^3 + n_z \, \gamma^2 \, \lambda \, \Omega - i \, \gamma \, (1 + \lambda^2) \, \Omega^2 + n_z \, \lambda \, (-1 + \lambda^2) \, \Omega^3 \right) \operatorname{Sin}[t \, \lambda \, \Omega] \right) \right) \right) / \\ & \quad \left( \gamma^6 + \gamma^4 \left( 3 + 2 \, \lambda^2 \right) \, \Omega^2 + \gamma^2 \left( 3 + \lambda^4 \right) \, \Omega^4 + (-1 + \lambda^2)^2 \, \Omega^6 \right) \left. \right] \end{aligned}$$

Yeah, Mathematica doesn't conjugate smartly. We have to outsmart Mathematica, below I do it by hand:

In[250]:= oUpDw =

$$\frac{1}{4} \times \left( -2 \, i \, e^{-t \gamma} \sin[t \, \Omega] - \left( 2 \, (n_x + i \, n_y) \, \gamma \left( n_z \, \gamma \left( -\gamma^4 - 2 \, \gamma^2 \, (1 + \lambda^2) \, \Omega^2 - (-1 + \lambda^2)^2 \, \Omega^4 \right) + \right. \right. \right. \\ \left. \left. \left( \gamma^2 + \Omega^2 \right) \left( -i \, \lambda \, \Omega \left( \gamma^2 + (-1 + \lambda^2) \, \Omega^2 \right) + n_z \, \gamma \left( \gamma^2 + (1 + \lambda^2) \, \Omega^2 \right) \right) \cos[t \, \lambda \, \Omega] + \right. \right. \\ \left. \left. e^{-t \gamma} \, \lambda \, \Omega \left( (i \, \gamma^4 + n_z \, \gamma^3 \, \lambda \, \Omega + i \, \gamma^2 \, \lambda^2 \, \Omega^2 + n_z \, \gamma \, \lambda \, (-3 + \lambda^2) \, \Omega^3 + i \, (-1 + \lambda^2) \, \Omega^4 \right) \right. \right. \\ \left. \left. \cos[t \, \Omega] + \Omega \left( -2 \, i \, \gamma^3 - 3 \, n_z \, \gamma^2 \, \lambda \, \Omega - 2 \, i \, \gamma \, \Omega^2 - n_z \, \lambda \, (-1 + \lambda^2) \, \Omega^3 \right) \sin[t \, \Omega] \right) + \right. \\ \left. \left. \left( \gamma^2 + \Omega^2 \right) \left( i \, \gamma^3 + n_z \, \gamma^2 \, \lambda \, \Omega + i \, \gamma \, (1 + \lambda^2) \, \Omega^2 + n_z \, \lambda \, (-1 + \lambda^2) \, \Omega^3 \right) \sin[t \, \lambda \, \Omega] \right) \right) \right) / \\ \left( \gamma^6 + \gamma^4 \, (3 + 2 \, \lambda^2) \, \Omega^2 + \gamma^2 \, (3 + \lambda^4) \, \Omega^4 + (-1 + \lambda^2)^2 \, \Omega^6 \right)$$

Out[250]=  $\frac{1}{4} \times$ 

$$\left( -2 \, i \, e^{-t \gamma} \sin[t \, \Omega] - \left( 2 \, (n_x + i \, n_y) \, \gamma \left( n_z \, \gamma \left( -\gamma^4 - 2 \, \gamma^2 \, (1 + \lambda^2) \, \Omega^2 - (-1 + \lambda^2)^2 \, \Omega^4 \right) + \left( \gamma^2 + \Omega^2 \right) \right. \right. \right. \\ \left. \left. \left( -i \, \lambda \, \Omega \left( \gamma^2 + (-1 + \lambda^2) \, \Omega^2 \right) + n_z \, \gamma \left( \gamma^2 + (1 + \lambda^2) \, \Omega^2 \right) \right) \cos[t \, \lambda \, \Omega] + \right. \right. \\ \left. \left. e^{-t \gamma} \, \lambda \, \Omega \left( (i \, \gamma^4 + n_z \, \gamma^3 \, \lambda \, \Omega + i \, \gamma^2 \, \lambda^2 \, \Omega^2 + n_z \, \gamma \, \lambda \, (-3 + \lambda^2) \, \Omega^3 + i \, (-1 + \lambda^2) \, \Omega^4 \right) \cos[t \, \Omega] + \right. \right. \\ \left. \left. \Omega \left( -2 \, i \, \gamma^3 - 3 \, n_z \, \gamma^2 \, \lambda \, \Omega - 2 \, i \, \gamma \, \Omega^2 - n_z \, \lambda \, (-1 + \lambda^2) \, \Omega^3 \right) \sin[t \, \Omega] \right) + \right. \\ \left. \left. \left( \gamma^2 + \Omega^2 \right) \left( i \, \gamma^3 + n_z \, \gamma^2 \, \lambda \, \Omega + i \, \gamma \, (1 + \lambda^2) \, \Omega^2 + n_z \, \lambda \, (-1 + \lambda^2) \, \Omega^3 \right) \sin[t \, \lambda \, \Omega] \right) \right) \right) / \\ \left( \gamma^6 + \gamma^4 \, (3 + 2 \, \lambda^2) \, \Omega^2 + \gamma^2 \, (3 + \lambda^4) \, \Omega^4 + (-1 + \lambda^2)^2 \, \Omega^6 \right)$$

In[251]:= oUpDwg =

$$- \left( \left( e^{-2 \, t \, \gamma - i \, t \, (-1 + \lambda) \, \Omega} \, (n_x + i \, n_y) \, \gamma \left( e^{2 \, t \, \gamma - i \, t \, \Omega} \, (-1 + n_z) \, (\gamma + i \, \Omega) \, (\gamma - i \, \Omega) \, (\gamma + i \, (-1 + \lambda) \, \Omega) \right. \right. \right. \\ \left. \left. \left( \gamma - i \, \lambda \, \Omega \right) \, (\gamma + i \, (1 + \lambda) \, \Omega) + e^{t \, (2 \, \gamma - i \, (1 - 2 \, \lambda) \, \Omega)} \, (1 + n_z) \, (\gamma + i \, \Omega) \right. \right. \\ \left. \left. \left( \gamma - i \, \Omega \right) \, (\gamma - i \, (-1 + \lambda) \, \Omega) \, (\gamma + i \, \lambda \, \Omega) \, (\gamma - i \, (1 + \lambda) \, \Omega) - \right. \right. \\ \left. \left. 2 \, e^{t \, (2 \, \gamma + i \, (-1 + \lambda) \, \Omega)} \, n_z \, \gamma \left( \gamma^2 + (-1 + \lambda)^2 \, \Omega^2 \right) \left( \gamma^2 + (1 + \lambda)^2 \, \Omega^2 \right) + \right. \right. \\ \left. \left. e^{t \, (\gamma + i \, \lambda \, \Omega)} \, \lambda \, (\gamma + i \, \Omega) \, \Omega \left( i \, \gamma + \Omega + n_z \, \lambda \, \Omega \right) \left( \gamma^2 + 2 \, i \, \gamma \, \Omega + (-1 + \lambda^2) \, \Omega^2 \right) + \right. \right. \\ \left. \left. e^{t \, (\gamma + i \, (-2 + \lambda) \, \Omega)} \, \lambda \, (\gamma - i \, \Omega) \, \Omega \left( i \, \gamma + (-1 + n_z \, \lambda) \, \Omega \right) \left( \gamma^2 - 2 \, i \, \gamma \, \Omega + (-1 + \lambda^2) \, \Omega^2 \right) \right) \right) \right) / \\ \left( 4 \, (\gamma^2 + \Omega^2) \left( \gamma^4 + 2 \, \gamma^2 \, (1 + \lambda^2) \, \Omega^2 + (-1 + \lambda^2)^2 \, \Omega^4 \right) \right)$$

Out[251]=  $- \left( \left( e^{-2 \, t \, \gamma - i \, t \, (-1 + \lambda) \, \Omega} \, (n_x + i \, n_y) \, \gamma \right. \right.$ 

$$\left. \left( e^{t \, (2 \, \gamma - i \, (1 - 2 \, \lambda) \, \Omega)} \, (1 + n_z) \, (\gamma - i \, \Omega) \, (\gamma + i \, \Omega) \, (\gamma - i \, (-1 + \lambda) \, \Omega) \, (\gamma + i \, \lambda \, \Omega) \right. \right. \\ \left. \left. \left( \gamma - i \, (1 + \lambda) \, \Omega \right) + e^{2 \, t \, \gamma - i \, t \, \Omega} \, (-1 + n_z) \, (\gamma - i \, \Omega) \, (\gamma + i \, \Omega) \, (\gamma + i \, (-1 + \lambda) \, \Omega) \, (\gamma - i \, \lambda \, \Omega) \right. \right. \\ \left. \left. \left( \gamma + i \, (1 + \lambda) \, \Omega \right) - 2 \, e^{t \, (2 \, \gamma + i \, (-1 + \lambda) \, \Omega)} \, n_z \, \gamma \left( \gamma^2 + (-1 + \lambda)^2 \, \Omega^2 \right) \left( \gamma^2 + (1 + \lambda)^2 \, \Omega^2 \right) + \right. \right. \\ \left. \left. e^{t \, (\gamma + i \, (-2 + \lambda) \, \Omega)} \, \lambda \, (\gamma - i \, \Omega) \, \Omega \left( i \, \gamma + (-1 + n_z \, \lambda) \, \Omega \right) \left( \gamma^2 - 2 \, i \, \gamma \, \Omega + (-1 + \lambda^2) \, \Omega^2 \right) + \right. \right. \\ \left. \left. e^{t \, (\gamma + i \, \lambda \, \Omega)} \, \lambda \, (\gamma + i \, \Omega) \, \Omega \left( i \, \gamma + \Omega + n_z \, \lambda \, \Omega \right) \left( \gamma^2 + 2 \, i \, \gamma \, \Omega + (-1 + \lambda^2) \, \Omega^2 \right) \right) \right) \right) / \\ \left( 4 \, (\gamma^2 + \Omega^2) \left( \gamma^4 + 2 \, \gamma^2 \, (1 + \lambda^2) \, \Omega^2 + (-1 + \lambda^2)^2 \, \Omega^4 \right) \right)$$

As it takes a lot of time to compute these overlaps I'll save them:

```
In[252]:= DumpSave["overlapsforSpinState.mx",
  {oUpUp, oDwDw, oDwUp, oUpDw, oUpUpg, oDwDwg, oDwUpg, oUpDwg}];
```

## b) Density matrix and fidelity: general analytics

```
In[ ]:= << AnalyticalExpressionOfTheFidelity.mx
```



$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{2} & \frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2} \end{pmatrix}$$

A generic density matrix of a qubit can be written as:

```
In[261]:= ρgen = Eye[2] + rx σx + ry σy + rz σz
           2 // mf;
```

$$\begin{pmatrix} \frac{1+rz}{2} & \frac{1}{2} (rx - i ry) \\ \frac{1}{2} (rx + i ry) & \frac{1-rz}{2} \end{pmatrix}$$

The fidelity is easily computed between our target (at time  $t=\pi/2r\Omega$ , with  $r=1$ ) and the general state:

```
In[262]:= F = QuantumFidelity[ρgen, ρtarget] // cf
```

```
Out[262]=  $\frac{1 - ry}{2}$ 
```

where

```
In[263]:= Tr[σy.ρgen] // cf
```

```
Out[263]= ry
```

```
In[266]:= ρtest =  $\begin{pmatrix} \rho_{uu} & \rho_{ud} \\ \rho_{du} & \rho_{dd} \end{pmatrix}$ ;
```

```
Tr[σy.ρtest] /. ρud → reρud + i imρud /. ρdu → reρud - i imρud // cf
```

```
Out[267]= -2 imρud
```

Hence,  $ry = -2 \operatorname{Im}\{\rho_{ud}\}$

So we have a way of obtaining an analytic expression for the fidelity, which is given by:

```
In[268]:= Im[Tr[σy.ρspin] // ComplexExpand]
```

```
Out[268]=
```

$$\operatorname{Im}\left[\dots 1 \dots\right] + \operatorname{Re}\left[-\frac{\dots 1 \dots}{4 \dots 2 \dots (\dots 1 \dots)} + \dots 12.874 \dots\right]$$

large output

show less

show more

show all

set size limit...

$$\text{In[269]:= } \mathcal{F}_{\text{analytical}} = \frac{1 - \text{Tr}[\sigma_y \cdot \rho_{\text{spin}}]}{2} \quad // \text{ cf}$$

$$\begin{aligned} \text{Out[269]= } & \left( e^{-t(\gamma + i\lambda\Omega)} \left( e^{2t(\gamma + i\lambda\Omega)} (-i n_x + n_y n_z) \gamma \right. \right. \\ & (\gamma - i\Omega) (\gamma + i\Omega) (\gamma - i(-1 + \lambda)\Omega) (\gamma + i\lambda\Omega) (\gamma - i(1 + \lambda)\Omega) + \\ & e^{2t\gamma} (n_x - i n_y n_z) \gamma (\gamma - i\Omega) (\gamma + i\Omega) (\gamma + i(-1 + \lambda)\Omega) (i\gamma + \lambda\Omega) (\gamma + i(1 + \lambda)\Omega) - \\ & 2 e^{2t\gamma + i t \lambda \Omega} \left( (-1 + n_y n_z) \gamma^2 - \Omega^2 \right) \left( \gamma^2 + (-1 + \lambda)^2 \Omega^2 \right) \left( \gamma^2 + (1 + \lambda)^2 \Omega^2 \right) - \\ & 2 e^{t(\gamma + i\lambda\Omega)} \left( \gamma^2 + \Omega^2 \right) \left( \gamma^2 + (-1 + \lambda)^2 \Omega^2 \right) \left( \gamma^2 + (1 + \lambda)^2 \Omega^2 \right) + \\ & e^{t(\gamma + i(-1 + \lambda)\Omega)} \gamma \lambda (\gamma - i\Omega) \Omega (n_x (\gamma + i\Omega) + n_y n_z \lambda \Omega) \left( \gamma^2 - 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2 \right) + \\ & \left. \left. e^{t(\gamma + i(1 + \lambda)\Omega)} \gamma \lambda (\gamma + i\Omega) \Omega (n_x (\gamma - i\Omega) + n_y n_z \lambda \Omega) \left( \gamma^2 + 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2 \right) \right) \right) / \\ & \left( 4 \times (-1 + e^{t\gamma}) \left( \gamma^2 + \Omega^2 \right) \left( \gamma^4 + 2 \gamma^2 (1 + \lambda^2) \Omega^2 + (-1 + \lambda^2)^2 \Omega^4 \right) \right) \end{aligned}$$

$$\text{In[270]:= } \mathcal{F}_{\text{tg}} = \mathcal{F}_{\text{analytical}} /. t \rightarrow \frac{\pi}{2\lambda\Omega} \quad // \text{ cf}$$

$$\begin{aligned} \text{Out[270]= } & - \left( \left( i e^{-\frac{\pi\gamma}{2\lambda\Omega}} \left( e^{\frac{\pi(\gamma - i\Omega)}{2\lambda\Omega}} \gamma \lambda \Omega (i\gamma + \Omega) (n_x (\gamma + i\Omega) + n_y n_z \lambda \Omega) \left( \gamma^2 - 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2 \right) - \right. \right. \right. \\ & 2 i e^{\frac{\pi\gamma}{2\lambda\Omega}} \left( \gamma^2 + \Omega^2 \right) \left( \gamma^4 + 2 \gamma^2 (1 + \lambda^2) \Omega^2 + (-1 + \lambda^2)^2 \Omega^4 \right) + 2 i e^{\frac{\pi\gamma}{\lambda\Omega}} \\ & \left( (1 + n_x - n_y n_z) \gamma^6 + n_y n_z \gamma^5 \lambda \Omega + \gamma^4 (3 + 2 \lambda^2 - 2 n_y n_z (1 + \lambda^2) + n_x (2 + \lambda^2)) \Omega^2 + \right. \\ & n_y n_z \gamma^3 \lambda^3 \Omega^3 + \gamma^2 (3 + \lambda^4 - n_y n_z (-1 + \lambda^2)^2 + n_x (1 + \lambda^2)) \Omega^4 + \\ & \left. \left. n_y n_z \gamma \lambda (-1 + \lambda^2) \Omega^5 + (-1 + \lambda^2)^2 \Omega^6 \right) + \right. \\ & \left. \left. e^{\frac{\pi(\gamma + i\Omega)}{2\lambda\Omega}} \gamma \lambda (\gamma + i\Omega) \Omega \left( \gamma^2 + 2 i \gamma \Omega + (-1 + \lambda^2) \Omega^2 \right) (i n_y n_z \lambda \Omega + n_x (i\gamma + \Omega)) \right) \right) / \\ & \left( 4 \times \left( -1 + e^{\frac{\pi\gamma}{2\lambda\Omega}} \right) \left( \gamma^2 + \Omega^2 \right) \left( \gamma^4 + 2 \gamma^2 (1 + \lambda^2) \Omega^2 + (-1 + \lambda^2)^2 \Omega^4 \right) \right) \end{aligned}$$

Let's save this nice expression:

`In[271]:= DumpSave["AnalyticalExpressionOfTheFidelity.mx", {Fanalytical, Ftg}];`

2) Fidelity for  $t_{\text{pulse}} = t_g = \pi / (2\Omega_g) = \pi / (2r_{\text{ge}}\Omega)$  ☒

3) Fidelity for  $t_{\text{pulse}} = t_{\text{optimal}}$  ☒

a) Finding  $t_{\text{optimal}}$

$$\begin{aligned} \text{In[807]:= } \text{Fidelity} = & \left( - \frac{n_y n_z \gamma^6}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} - \right. \\ & \frac{n_y n_z \gamma^4 \Omega e^2}{(\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} - \\ & \frac{n_y n_z \gamma^2 \Omega e^4}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} - \\ & \left. \frac{n_y n_z \gamma^4 \Omega g^2}{(\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \right) \end{aligned}$$

$$\begin{aligned}
& \frac{ny \, nz \, \gamma^2 \, \Omega e^2 \, \Omega g^2}{(\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} - \\
& \frac{ny \, nz \, \gamma^2 \, \Omega g^4}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{ny \, nz \, \gamma^6 \, \text{Cos}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{ny \, nz \, \gamma^4 \, \Omega e^2 \, \text{Cos}[T \, \Omega g]}{(\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{ny \, nz \, \gamma^2 \, \Omega e^4 \, \text{Cos}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} - \\
& \frac{nx \, \gamma^5 \, \Omega g \, \text{Cos}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{nx \, \gamma \, \Omega e^4 \, \Omega g \, \text{Cos}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{ny \, nz \, \gamma^4 \, \Omega g^2 \, \text{Cos}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{ny \, nz \, \gamma^2 \, \Omega e^2 \, \Omega g^2 \, \text{Cos}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} - \\
& \frac{nx \, \gamma^3 \, \Omega g^3 \, \text{Cos}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} - \\
& \frac{nx \, \gamma \, \Omega e^2 \, \Omega g^3 \, \text{Cos}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{nx \, \gamma^6 \, \text{Sin}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{nx \, \gamma^4 \, \Omega e^2 \, \text{Sin}[T \, \Omega g]}{(\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{nx \, \gamma^2 \, \Omega e^4 \, \text{Sin}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{ny \, nz \, \gamma^5 \, \Omega g \, \text{Sin}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} - \\
& \frac{ny \, nz \, \gamma \, \Omega e^4 \, \Omega g \, \text{Sin}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{nx \, \gamma^4 \, \Omega g^2 \, \text{Sin}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} + \\
& \frac{nx \, \gamma^2 \, \Omega e^2 \, \Omega g^2 \, \text{Sin}[T \, \Omega g]}{2 (\gamma^2 + \Omega e^2) (\gamma^2 + (\Omega e - \Omega g)^2) (\gamma^2 + (\Omega e + \Omega g)^2)} +
\end{aligned}$$

$$\left. \begin{aligned} & \frac{ny \, nz \, \gamma^3 \, \Omega g^3 \, \text{Sin}[T \, \Omega g]}{2 \, (\gamma^2 + \Omega e^2) \, (\gamma^2 + (\Omega e - \Omega g)^2) \, (\gamma^2 + (\Omega e + \Omega g)^2)} + \\ & \frac{ny \, nz \, \gamma \, \Omega e^2 \, \Omega g^3 \, \text{Sin}[T \, \Omega g]}{2 \, (\gamma^2 + \Omega e^2) \, (\gamma^2 + (\Omega e - \Omega g)^2) \, (\gamma^2 + (\Omega e + \Omega g)^2)} \end{aligned} \right) /. \gamma \rightarrow 1 // \text{Simplify}$$

$$\begin{aligned} \text{Out}[807]= & \left( -ny \, nz \, (\Omega e^4 - 2 \, \Omega e^2 \, (-1 + \Omega g^2) + (1 + \Omega g^2)^2) + \right. \\ & (1 + \Omega e^2) \, (nx \, \Omega g \, (-1 + \Omega e^2 - \Omega g^2) + ny \, nz \, (1 + \Omega e^2 + \Omega g^2)) \, \text{Cos}[T \, \Omega g] + \\ & (1 + \Omega e^2) \, (nx \, (1 + \Omega e^2 + \Omega g^2) + ny \, nz \, (\Omega g - \Omega e^2 \, \Omega g + \Omega g^3)) \, \text{Sin}[T \, \Omega g] \left. \right) / \\ & (2 \times (1 + \Omega e^2) \times (1 + \Omega e^2 - 2 \, \Omega e \, \Omega g + \Omega g^2) \times (1 + \Omega e^2 + 2 \, \Omega e \, \Omega g + \Omega g^2)) \end{aligned}$$

$$\text{In}[811]:= \text{approx}f = \text{Fidelity} /. \{\Omega e^2 \rightarrow 0, \Omega g^2 \rightarrow 0, \Omega e \, \Omega g \rightarrow 0, \Omega e^4 \rightarrow 0\}$$

(\*Get rid of all the higher order terms\*)

$$\text{Out}[811]= \frac{1}{2} \left( -ny \, nz + (ny \, nz - nx \, \Omega g) \, \text{Cos}[T \, \Omega g] + (nx + ny \, nz \, (\Omega g + \Omega g^3)) \, \text{Sin}[T \, \Omega g] \right)$$

$$\text{sol} = \text{Solve}[D[\text{approx}f, T] == 0, T]$$

$$\left\{ \left\{ T \rightarrow \text{ConditionalExpression} \left[ \frac{1}{\Omega g} \left( \text{ArcTan} \left[ -\frac{ny \, nz - nx \, \Omega g}{\sqrt{nx^2 + ny^2 \, nz^2 + nx^2 \, \Omega g^2 + ny^2 \, nz^2 \, \Omega g^2}} \right. \right. \right. \right. \right. \\ \left. \left. \left. \frac{nx \, ny \, nz}{\sqrt{(nx^2 + ny^2 \, nz^2) \, (1 + \Omega g^2)}} - \frac{nx^2 \, \Omega g}{\sqrt{(nx^2 + ny^2 \, nz^2) \, (1 + \Omega g^2)}} + \frac{ny^2 \, nz^2 \, \Omega g}{\sqrt{(nx^2 + ny^2 \, nz^2) \, (1 + \Omega g^2)}} - \frac{nx \, ny \, nz \, \Omega g^2}{\sqrt{(nx^2 + ny^2 \, nz^2) \, (1 + \Omega g^2)}} \right. \right. \right. \\ \left. \left. \left. - ny \, nz + nx \, \Omega g \right. \right. \right. \right. \\ \left. \left. + 2 \, \pi \, C[1] \right) \right], C[1] \in \text{Integers} \right\},$$

$$\left\{ T \rightarrow \text{ConditionalExpression} \left[ \frac{1}{\Omega g} \left( \text{ArcTan} \left[ \frac{ny \, nz - nx \, \Omega g}{\sqrt{nx^2 + ny^2 \, nz^2 + nx^2 \, \Omega g^2 + ny^2 \, nz^2 \, \Omega g^2}} \right. \right. \right. \right. \right. \\ \left. \left. \left. - \frac{nx \, ny \, nz}{\sqrt{(nx^2 + ny^2 \, nz^2) \, (1 + \Omega g^2)}} + \frac{nx^2 \, \Omega g}{\sqrt{(nx^2 + ny^2 \, nz^2) \, (1 + \Omega g^2)}} - \frac{ny^2 \, nz^2 \, \Omega g}{\sqrt{(nx^2 + ny^2 \, nz^2) \, (1 + \Omega g^2)}} + \frac{nx \, ny \, nz \, \Omega g^2}{\sqrt{(nx^2 + ny^2 \, nz^2) \, (1 + \Omega g^2)}} \right. \right. \right. \\ \left. \left. \left. - ny \, nz + nx \, \Omega g \right. \right. \right. \right. \\ \left. \left. + 2 \, \pi \, C[1] \right) \right], C[1] \in \text{Integers} \right\} \right\}$$

T /. sol /. {nx^2 ny^2 → 0, nx^2 nz^2 → 0, nz^2 ny^2 → 0}

$$\left\{ \text{ConditionalExpression} \left[ \frac{\text{ArcTan} \left[ -\frac{ny \, nz - nx \, \Omega g}{\sqrt{nx^2 + nx^2 \, \Omega g^2}}, \frac{\frac{nx \, ny \, nz}{\sqrt{nx^2 (1 + \Omega g^2)}} - \frac{nx^2 \, \Omega g}{\sqrt{nx^2 (1 + \Omega g^2)}} - \frac{nx \, ny \, nz \, \Omega g^2}{\sqrt{nx^2 (1 + \Omega g^2)}}}{-ny \, nz + nx \, \Omega g} \right] + 2 \pi C[1]}{\Omega g}, \right. \\ \left. C[1] \in \text{Integers} \right], \text{ConditionalExpression} \left[ \frac{\text{ArcTan} \left[ \frac{ny \, nz - nx \, \Omega g}{\sqrt{nx^2 + nx^2 \, \Omega g^2}}, \frac{-\frac{nx \, ny \, nz}{\sqrt{nx^2 (1 + \Omega g^2)}} + \frac{nx^2 \, \Omega g}{\sqrt{nx^2 (1 + \Omega g^2)}} + \frac{nx \, ny \, nz \, \Omega g^2}{\sqrt{nx^2 (1 + \Omega g^2)}}}{-ny \, nz + nx \, \Omega g} \right] + 2 \pi C[1]}{\Omega g}, C[1] \in \text{Integers} \right] \} \\ \text{trial} = \frac{\text{ArcTan} \left[ -\frac{ny \, nz - nx \, \Omega g}{\sqrt{nx^2 + nx^2 \, \Omega g^2}}, \frac{\frac{nx \, ny \, nz}{\sqrt{nx^2 (1 + \Omega g^2)}} - \frac{nx^2 \, \Omega g}{\sqrt{nx^2 (1 + \Omega g^2)}} - \frac{nx \, ny \, nz \, \Omega g^2}{\sqrt{nx^2 (1 + \Omega g^2)}}}{-ny \, nz + nx \, \Omega g} \right]}{\Omega g} // \text{FullSimplify} \\ \frac{\text{ArcTan} \left[ \frac{-ny \, nz + nx \, \Omega g}{\sqrt{nx^2 (1 + \Omega g^2)}}, -\frac{nx (nx \, \Omega g + ny \, nz (-1 + \Omega g^2))}{(-ny \, nz + nx \, \Omega g) \sqrt{nx^2 (1 + \Omega g^2)}} \right]}{\Omega g}$$

Fidelity /. {T → Pi / Ωg - ArcTan[nx / (nx Ωg - ny nz)] / Ωg}

$$\left( -ny \, nz \left( \Omega e^4 - 2 \Omega e^2 (-1 + \Omega g^2) + (1 + \Omega g^2)^2 \right) + \right. \\ \left. (1 + \Omega e^2) (nx \, \Omega g (-1 + \Omega e^2 - \Omega g^2) + ny \, nz (1 + \Omega e^2 + \Omega g^2)) \right. \\ \left. \cos \left[ \Omega g \left( \frac{\pi}{\Omega g} - \frac{\text{ArcTan} \left[ \frac{nx}{-ny \, nz + nx \, \Omega g} \right]}{\Omega g} \right) \right] + (1 + \Omega e^2) \right. \\ \left. (ny \, nz \, \Omega g (1 - \Omega e^2 + \Omega g^2) + nx (1 + \Omega e^2 + \Omega g^2)) \sin \left[ \Omega g \left( \frac{\pi}{\Omega g} - \frac{\text{ArcTan} \left[ \frac{nx}{-ny \, nz + nx \, \Omega g} \right]}{\Omega g} \right) \right] \right) / \\ (2 \times (1 + \Omega e^2) \times (1 + \Omega e^2 - 2 \Omega e \, \Omega g + \Omega g^2) \times (1 + \Omega e^2 + 2 \Omega e \, \Omega g + \Omega g^2))$$

## b) Analytical expression and plots

Components of the fidelity as a function of time is given by:



In[738]:=

$$\Omega s = \left\{ \Delta \Omega m \rightarrow \frac{(\Omega g - \Omega e)}{2}, \Delta \Omega p \rightarrow \frac{(\Omega g + \Omega e)}{2} \right\};$$

$$f_{xt} = \frac{1 + (\Omega e / \gamma)^2 + (\Omega g / \gamma)^2}{\left(1 + 4 \left(\frac{\Delta \Omega m}{\gamma}\right)^2\right) \times \left(1 + 4 \left(\frac{\Delta \Omega p}{\gamma}\right)^2\right)} \sin[\Omega g t] -$$

$$\frac{1 - (\Omega e / \gamma)^2 + (\Omega g / \gamma)^2}{\left(1 + 4 \left(\frac{\Delta \Omega m}{\gamma}\right)^2\right) \times \left(1 + 4 \left(\frac{\Delta \Omega p}{\gamma}\right)^2\right)} \frac{\Omega g}{\gamma} \cos[\Omega g t] /. \Omega s /. \Omega e \rightarrow \Omega /. \Omega g \rightarrow \lambda \Omega // cf;$$

$$f_{yzt} = \frac{(\Omega g / \gamma) \sin[\Omega g t] - 1 - 2 \left(\frac{\Omega e}{\gamma}\right)^2 - 2 \left(\frac{\Omega g}{\gamma}\right)^2}{\left(1 + \left(\frac{\Omega e}{\gamma}\right)^2\right) \times \left(1 + 4 \left(\frac{\Delta \Omega m}{\gamma}\right)^2\right) \times \left(1 + 4 \left(\frac{\Delta \Omega p}{\gamma}\right)^2\right)} +$$

$$\frac{1 + \left(\frac{\Omega e}{\gamma}\right)^2 + \left(\frac{\Omega g}{\gamma}\right)^2}{\left(1 + 4 \left(\frac{\Delta \Omega m}{\gamma}\right)^2\right) \times \left(1 + 4 \left(\frac{\Delta \Omega p}{\gamma}\right)^2\right)} \cos[\Omega g t] /. \Omega s /. \Omega e \rightarrow \Omega /. \Omega g \rightarrow \lambda \Omega // cf;$$

In[741]:=

$$t_{optimal} = \frac{\pi}{\Omega g} - \frac{1}{\Omega g} \text{ArcTan}\left[\frac{n_x}{n_x \Omega g - n_y n_z}\right] /. \Omega e \rightarrow \Omega /. \Omega g \rightarrow \lambda \Omega;$$

The fidelity as a function of time is given by:

In[742]:=

$$\mathcal{F}t = \frac{1}{2} - \frac{n_y n_z}{2} f_{yzt} + \frac{n_x}{2} f_{xt} // cf$$

Out[742]=

$$\frac{1}{2} \times \left( 1 + \frac{n_x \gamma (-\lambda \Omega (\gamma^2 + (-1 + \lambda^2) \Omega^2) \cos[t \lambda \Omega] + \gamma (\gamma^2 + (1 + \lambda^2) \Omega^2) \sin[t \lambda \Omega])}{\gamma^4 + 2 \gamma^2 (1 + \lambda^2) \Omega^2 + (-1 + \lambda^2)^2 \Omega^4} + \right.$$

$$\left. \frac{(n_y n_z \gamma^2 (- (\gamma^2 + \Omega^2) (\gamma^2 + (1 + \lambda^2) \Omega^2) \cos[t \lambda \Omega]) + \gamma^2 (\gamma^2 + 2 \times (1 + \lambda^2) \Omega^2 - \gamma \lambda \Omega \sin[t \lambda \Omega]))}{((\gamma^2 + \Omega^2) (\gamma^2 + (-1 + \lambda^2)^2 \Omega^2) (\gamma^2 + (1 + \lambda^2)^2 \Omega^2))} \right)$$

In[743]:=

$$\mathcal{F}t_{optimal} = \mathcal{F}t /. t \rightarrow t_{optimal};$$

In[744]:=

$$\mathcal{F}\lambda\Omega 2 = \mathcal{F}t_{optimal} /. idealalignmentparamaters // cf$$

Out[744]=

$$\frac{1}{2} \times \left( 1 + \frac{1 + \Omega^2 (1 + \lambda^2 (2 + (-1 + \lambda^2) \Omega^2))}{\sqrt{1 + \lambda^2 \Omega^2} (1 + 2 \times (1 + \lambda^2) \Omega^2 + (-1 + \lambda^2)^2 \Omega^4)} \right)$$

```

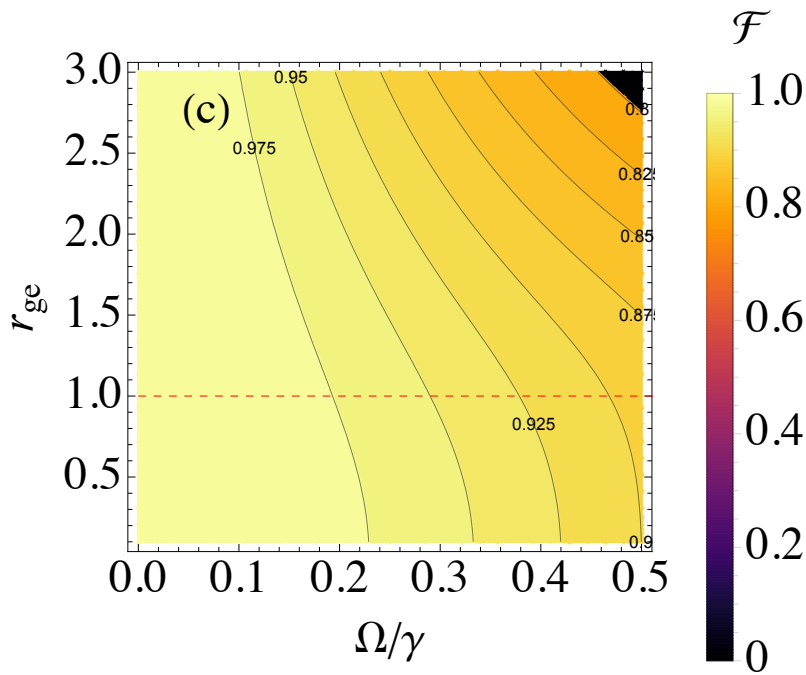
In[745]:= Module[{cf},

  cf = MPLColorMap["Inferno"];

  plot3 =
    ContourPlot[ $\mathcal{F} \lambda \Omega^2$ , { $\Omega$ , 0., 0.5}, { $\lambda$ , 0.1, 3.},
      PlotRange → All,
      AspectRatio → 7 / 7.5,
      FrameLabel → {Style[" $\Omega/\gamma$ ", FontFamily → "Times", FontSize → fontsize, Black],
        Style[" $r_{ge}$ ", FontFamily → "Times", FontSize → fontsize, Black]},
      LabelStyle → Directive[FontFamily → "Times", FontSize → fontsize, Black],
      ColorFunction → cf, ContourLabels → All, ColorFunctionScaling → False,
      PlotLegends → Placed[BarLegend[{cf, {0, 1}}, LegendLabel → Style[" $\mathcal{F}$ ",
        FontFamily → "Times", FontSize → fontsize, Black]], Right], Epilog → {
        {Text[Style["(c)", FontSize → fontsize, FontFamily → "Times",
          FontColor → Black], Scaled[{0.15, 0.9}]]},
        (*Horizontal line*) {Red, Dashed, Line[{{0, 1}, {1, 1}}]}},
      ImageSize → 350]
]

```

Out[745]=



```

In[559]:= λλlist = {1.0, 1.5, 2.5};
Module[{nhathat, parOptimal, xhat},
  nhathat = Normalize@{1, nn, nn};
  xhat = {1, 0, 0};
  parOptimal = {γ → 1, t → toptimal, λ → λλ,
    nx → N[nhathat[[1]]], ny → N[nhathat[[2]]], nz → N[nhathat[[3]]], Ω → ΩΩ};
  Do[

    fidelitytOptimalcontplot[λλ] =
      Flatten[Table[{nhathat.xhat, N@ΩΩ, Chop@N[ℱtoptimal /. parOptimal]},
        {ΩΩ, 10-2, 0.5, 10-3}, {nn, 0, 0.8, 10-2}], 1]

    , {λλ, λλlist}]
]

In[561]:= λλlist = {1.0, 1.5, 2.5};
Module[{nhathat, partg, xhat},
  nhathat = Normalize@{1, nn, nn};
  xhat = {1, 0, 0};
  partg = {γ → 1, t → π / (2 λ Ω), λ → λλ,
    nx → N[nhathat[[1]]], ny → N[nhathat[[2]]], nz → N[nhathat[[3]]], Ω → ΩΩ};
  Do[

    fidelitytgcontplot[λλ] = Flatten[Table[{nhathat.xhat, N@ΩΩ, Chop@N[ℱch /. partg]},
      {ΩΩ, 10-2, 0.5, 10-3}, {nn, 0, 0.8, 10-2}], 1]

    , {λλ, λλlist}]
]

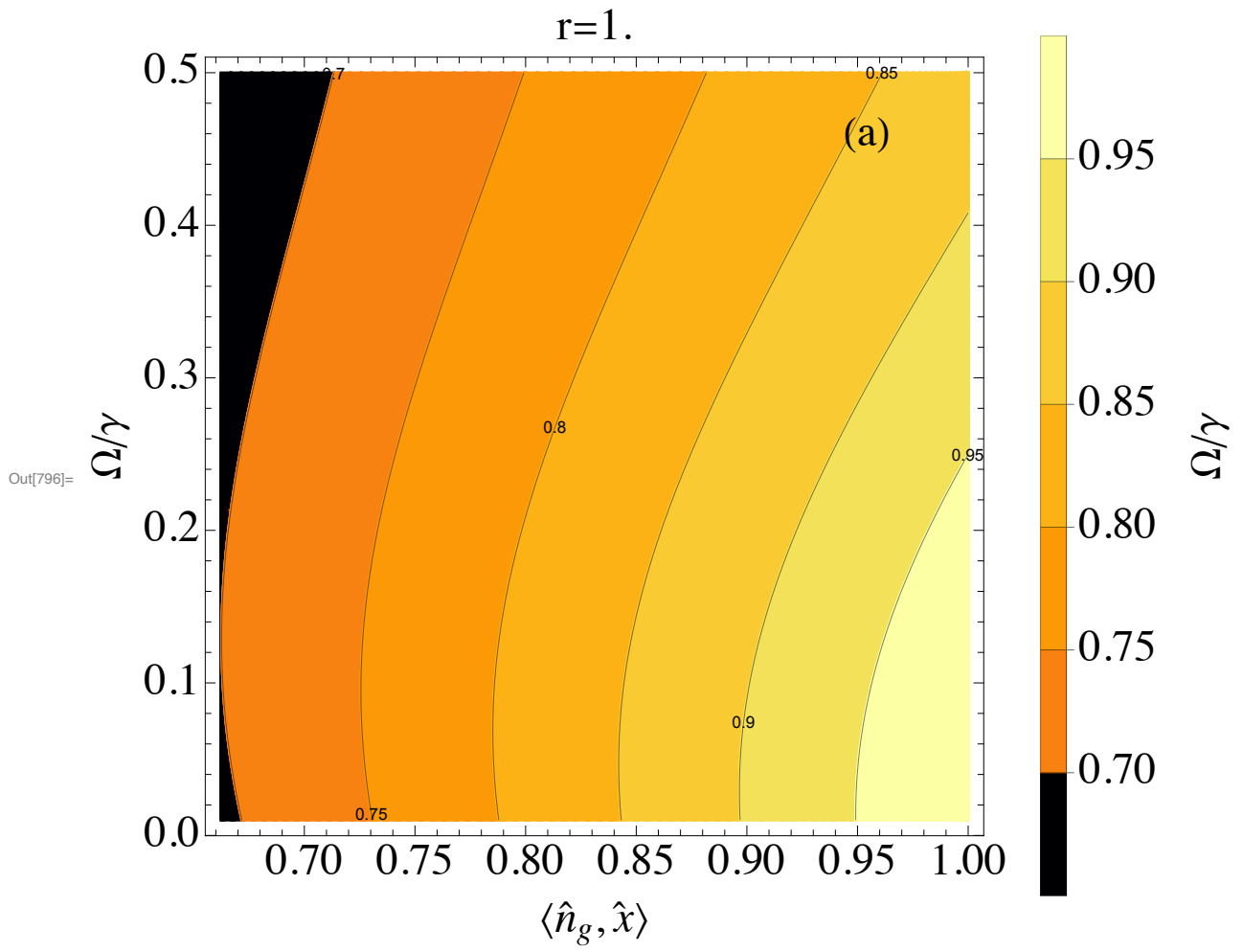
```

```

In[796]:= Module[{cf, plotSize, frameLabelStyle},

  cf = MPLColorMap["Inferno"];
  plotSize = 500;
  frameLabelStyle =
    {FontSize → fontsize, FontColor → Black, FontFamily → "Times"};
  contourplotsInnerProdTg = Grid[{Table[
    ListContourPlot[fidelitytgcontplot[ $\lambda$ list[[j]]],
    PlotRange → All, FrameLabel →
      {Style[" $\langle \hat{n}_g, \hat{x} \rangle$ ", FontFamily → "Times", FontSize → fontsize, Black],
       Style[" $\Omega/\gamma$ ", FontFamily → "Times", FontSize → fontsize, Black]},
    LabelStyle → Directive[FontFamily → "Times", FontSize → fontsize, Black],
    ColorFunction → cf, ContourLabels → All, ColorFunctionScaling → False,
    ImageSize → plotSize,
    Epilog → {Text[Style[alphabetlabel[[j]], FontSize → fontsize,
      FontFamily → "Times", FontColor → Black], Scaled[{0.85, 0.9}]]},
    PlotLegends → Automatic, PlotLabel → Style["r=" <> ToString[ $\lambda$ list[[j]]],
      FontSize → fontsize, FontFamily → "Times", FontColor → Black]
  ]
  , {j, 1, Length@ $\lambda$ list}]]]
]
savePlot["Fidelity-ContPlot-InnerProdTg.jpg", contourplotsInnerProdTg]

```

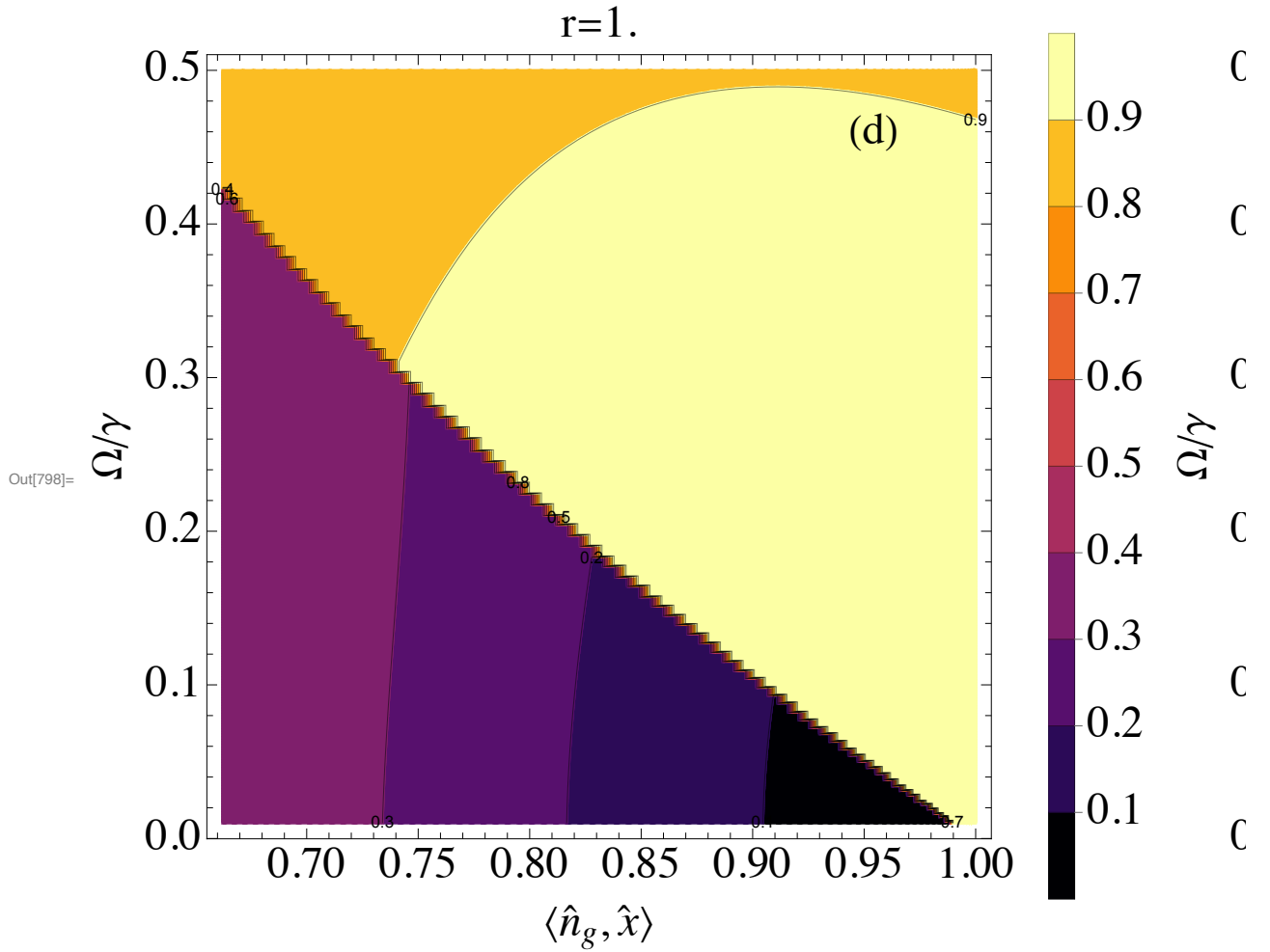


```

In[798]:= Module[{cf, plotSize, frameLabelStyle},

  cf = MPLColorMap["Inferno"];
  plotSize = 500;
  frameLabelStyle =
    {FontSize → fontsize, FontColor → Black, FontFamily → "Times"};
  contourplotsInnerProdTOptimal = Grid[{Table[
    ListContourPlot[fidelitytOptimalcontplot[ $\lambda$ list[[j]]],
    PlotRange → All, FrameLabel →
      {Style[" $\langle \hat{n}_g, \hat{x} \rangle$ ", FontFamily → "Times", FontSize → fontsize, Black],
       Style[" $\Omega/\gamma$ ", FontFamily → "Times", FontSize → fontsize, Black]},
    LabelStyle → Directive[FontFamily → "Times", FontSize → fontsize, Black],
    ColorFunction → cf, ContourLabels → All, ColorFunctionScaling → False,
    ImageSize → plotSize,
    Epilog → {Text[Style[alphabetlabel[[j + 3]], FontSize → fontsize,
      FontFamily → "Times", FontColor → Black], Scaled[{0.85, 0.9}]]},
    PlotLegends → Automatic, PlotLabel → Style["r=" <> ToString[ $\lambda$ list[[j]]],
      FontSize → fontsize, FontFamily → "Times", FontColor → Black]
  ]
  , {j, 1, Length@ $\lambda$ list}]]]
]
savePlot["Fidelity-ContPlot-InnerProdTOptimal.jpg",
  contourplotsInnerProdTOptimal]

```



## IV. Spin decoupling ✓

### 1) Analytics for Intensities and cBhat ✓

```
In[577]:= IRUpSE = γ Abs[f0SE["e", "upm", "e", "upm", t]]^2 // cf
IRDwSE = γ Abs[f0SE["e", "upm", "e", "dwm", t]]^2 // cf

ILUpSE = γ Abs[f0SE["e", "dwm", "e", "upm", t]]^2 // cf
ILDwSE = γ Abs[f0SE["e", "dwm", "e", "dwm", t]]^2 // cf
```

$$\text{Out[577]= } e^{-t\gamma} \gamma \cos\left[\frac{t\Omega}{2}\right]^2$$

$$\text{Out[578]= } e^{-t\gamma} \gamma \sin\left[\frac{t\Omega}{2}\right]^2$$

$$\text{Out[579]= } e^{-t\gamma} \gamma \sin\left[\frac{t\Omega}{2}\right]^2$$

$$\text{Out[580]= } e^{-t\gamma} \gamma \cos\left[\frac{t\Omega}{2}\right]^2$$

In[581]:= **IRUpSE**

$$\text{Out[581]} = e^{-t\gamma} \gamma \cos\left[\frac{t\Omega}{2}\right]^2$$

In[582]:= **pRUUp = Integrate[IRUpSE, {t, 0, \tau}]**

$$\text{Out[582]} = \frac{1}{4} \gamma \left( \frac{2 - 2e^{-\gamma\tau}}{\gamma} + \frac{1 - e^{-\tau(\gamma - i\Omega)}}{\gamma - i\Omega} + \frac{1 - e^{-\tau(\gamma + i\Omega)}}{\gamma + i\Omega} \right)$$

In[583]:= **% // cf**

$$\text{Out[583]} = \frac{1}{2(\gamma^2 + \Omega^2)} e^{-\gamma\tau} \left( (-1 + 2e^{\gamma\tau}) \gamma^2 + (-1 + e^{\gamma\tau}) \Omega^2 - \gamma^2 \cos[\tau\Omega] + \gamma\Omega \sin[\tau\Omega] \right)$$

In[584]:= **% // Expand**

$$\text{Out[584]} = \frac{\gamma^2}{\gamma^2 + \Omega^2} - \frac{e^{-\gamma\tau} \gamma^2}{2(\gamma^2 + \Omega^2)} + \frac{\Omega^2}{2(\gamma^2 + \Omega^2)} - \frac{e^{-\gamma\tau} \Omega^2}{2(\gamma^2 + \Omega^2)} - \frac{e^{-\gamma\tau} \gamma^2 \cos[\tau\Omega]}{2(\gamma^2 + \Omega^2)} + \frac{e^{-\gamma\tau} \gamma\Omega \sin[\tau\Omega]}{2(\gamma^2 + \Omega^2)}$$

Assuming  $\gamma\tau \gg 1$ , we neglect the exponential terms (SS stands for steady state):

$$\text{In[585]} = \text{pRUUpSS} = \frac{\gamma^2}{\gamma^2 + \Omega^2} + \frac{\Omega^2}{2(\gamma^2 + \Omega^2)} \left( * - \frac{e^{-\gamma\tau} \gamma^2 \cos[\tau\Omega]}{2(\gamma^2 + \Omega^2)} + \frac{e^{-\gamma\tau} \gamma\Omega \sin[\tau\Omega]}{2(\gamma^2 + \Omega^2)} - \frac{e^{-\gamma\tau} \gamma^2}{2(\gamma^2 + \Omega^2)} - \frac{e^{-\gamma\tau} \Omega^2}{2(\gamma^2 + \Omega^2)} * \right) // \text{cf}$$

$$\text{Out[585]} = \frac{1}{2} \times \left( 1 + \frac{\gamma^2}{\gamma^2 + \Omega^2} \right)$$

In[586]:= **cBhatSE = 2 \sqrt{pRUUpSS (1 - pRUUpSS)} // cf**

$$\text{Out[586]} = \frac{\Omega \sqrt{2\gamma^2 + \Omega^2}}{\gamma^2 + \Omega^2}$$

Expanding in Taylor series for  $\Omega$  close to 0:

In[588]:= **Series[cBhatSE, {\Omega, 0, 10}]**

$$\text{Out[588]} = \frac{\sqrt{2}\Omega}{\gamma} - \frac{3\Omega^3}{2(\sqrt{2}\gamma^3)} + \left( -\frac{9}{16\sqrt{2}\gamma^5} + \frac{\sqrt{2}}{\gamma^5} \right) \Omega^5 + \left( \frac{37}{64\sqrt{2}\gamma^7} - \frac{\sqrt{2}}{\gamma^7} \right) \Omega^7 + \left( -\frac{597}{1024\sqrt{2}\gamma^9} + \frac{\sqrt{2}}{\gamma^9} \right) \Omega^9 + O[\Omega]^{11}$$



```

In[714]:= cBhatPlot = Plot[cBhatSE /.  $\gamma \rightarrow 1$ , { $\Omega$ , 0, 0.5},
  AspectRatio  $\rightarrow$  10 / 20,
  PlotRange  $\rightarrow$  {{0, 0.51}, {0, 1}},
  PlotStyle  $\rightarrow$  {red},
  FrameLabel  $\rightarrow$  {" $\Omega/\gamma$ ", " $B_{cl}$ "}]
(*Save the figure in every project it is used.*)
savePlot["cBhatPlot.pdf", cBhatPlot]

```

