Computational Physics – Exercise 9: Spin-1/2 & Nuclear magnetic resonance

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Exercise: Rotation of magnetization

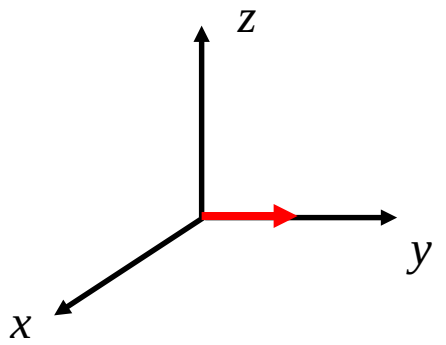
- Solve the Bloch equation for

$$\vec{B}(t) = (h\cos\omega_0 t, -h\sin\omega_0 t, B^0), \quad 1/T_1 = 1/T_2 = 0, \quad \vec{M}(t=0) = (0,1,0)$$

$$B^0 = 2\pi f_0, \quad f_0 = 4$$

$$h = 2\pi f_1, \quad f_1 = 1/4$$

$$\gamma = 1 \rightarrow \omega_0 = B^0$$



→ For $t = 1$ a $\pi/2$ rotation is made:

$$\vec{M}(t=0) = (0,1,0) \rightarrow \vec{M}(t=1) = (0,0,-1)$$

Use 100 steps to "resolve" f_0

Repeat for more time steps to see the time evolution

Plot $M^x(t), M^y(t), M^z(t)$

Exercise: Rotation of magnetization

- Repeat the calculation for $1/T_1 = 0, 1/T_2 = 1$
- Repeat the calculation for $1/T_1 = 1, 1/T_2 = 0$
- Repeat the calculation for $1/T_1 = 1/T_2 = 1$
- Repeat the calculation for other rotations and different begin orientation:

  e.g. $\vec{B}(t) = (h\cos(\omega_0 t + \varphi), -h\sin(\omega_0 t + \varphi), B^0)$ with

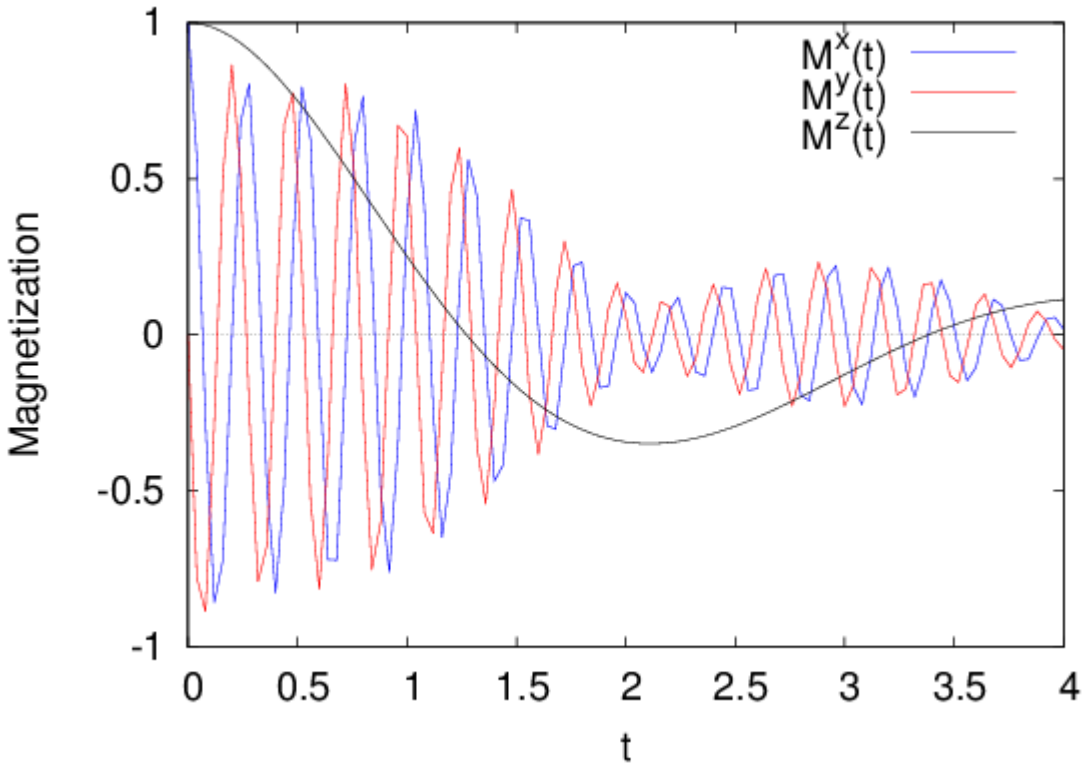
  $\varphi = \pi/2$ or $\varphi = \pi/4$ and $\vec{M}(t=0) = (1,0,0)$

  $= (0,0,1)$

  $= (1,0,1)$

Exercise: Rotation of magnetization

- Example for $1/T_1 = 0, 1/T_2 = 1$ and $\vec{M}(t=0) = (1,0,1)$



Report

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- Filename: Report_9_Surname1_Surname2.pdf, where Surname1 < Surname02 (alphabetical order). Example: Report_9_Jin_Lagemann.pdf (Do not use “umlauts” or any other special characters in the names)
- Content of the report:
  - Names + matricle numbers + e-mail addresses + title
  - Introduction: describe briefly the problem you are modeling and simulating (write in complete sentences)
  - Simulation model and method: describe briefly the model and simulation method (write in complete sentences)
  - Simulation results: show figures (use grids, with figure captions !) depicting the simulation results. Give a brief description of the results (write in complete sentences)
  - Discussion: summarize your findings
  - Appendix: Include the listing of the program

Due date: 5 PM, July 7, 2020

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