Mechanical Bloch equations.

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Abstract

Walking through the paper *(2014, Frimmer and Novotny) "The classical Bloch equations"* [1][1] and the book *(2010, Smith) "Waves and Oscillations: A Prelude to Quantum Mechanics"* [2].

Contents

1 Setup

```
Python

import pennylane as qml
import numpy as np
import matplotlib.pyplot as plt
```

[1]Preprint: https://arxiv.org/abs/1410.0710

2 Following the book

(2010, Smith) "Waves and Oscillations: A Prelude to Quantum Mechanics" [2].

2.1 Coupled oscillators

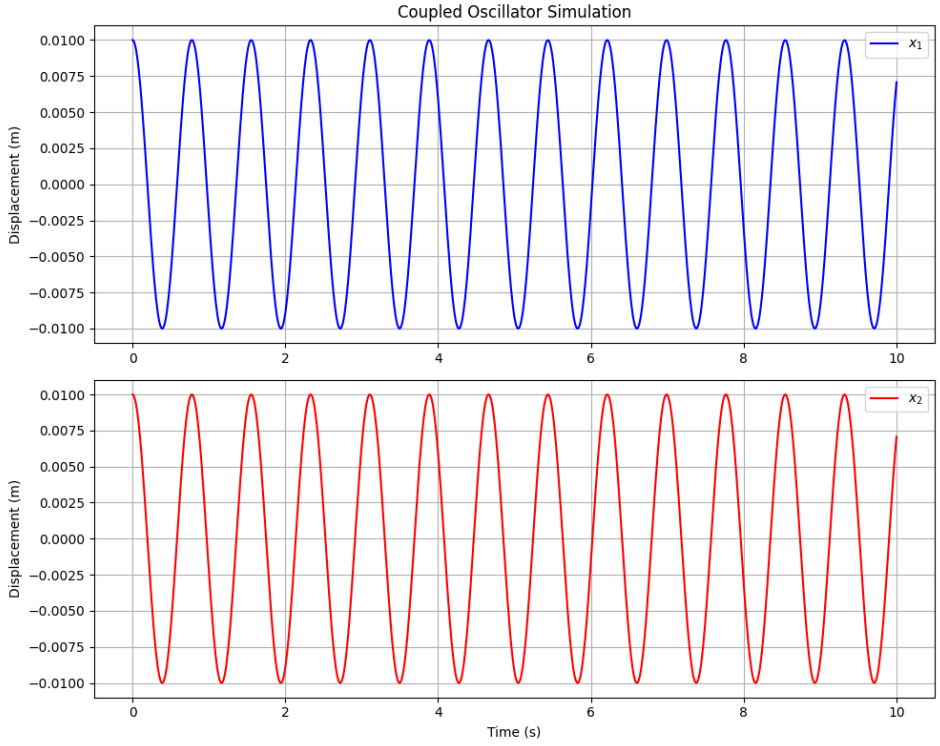
$$\ddot{x}_1 + \frac{g}{\ell}x_1 + \frac{k}{m}(x_1 - x_2) = 0,$$
$$\ddot{x}_2 + \frac{g}{\ell}x_2 + \frac{k}{m}(x_2 - x_1) = 0$$

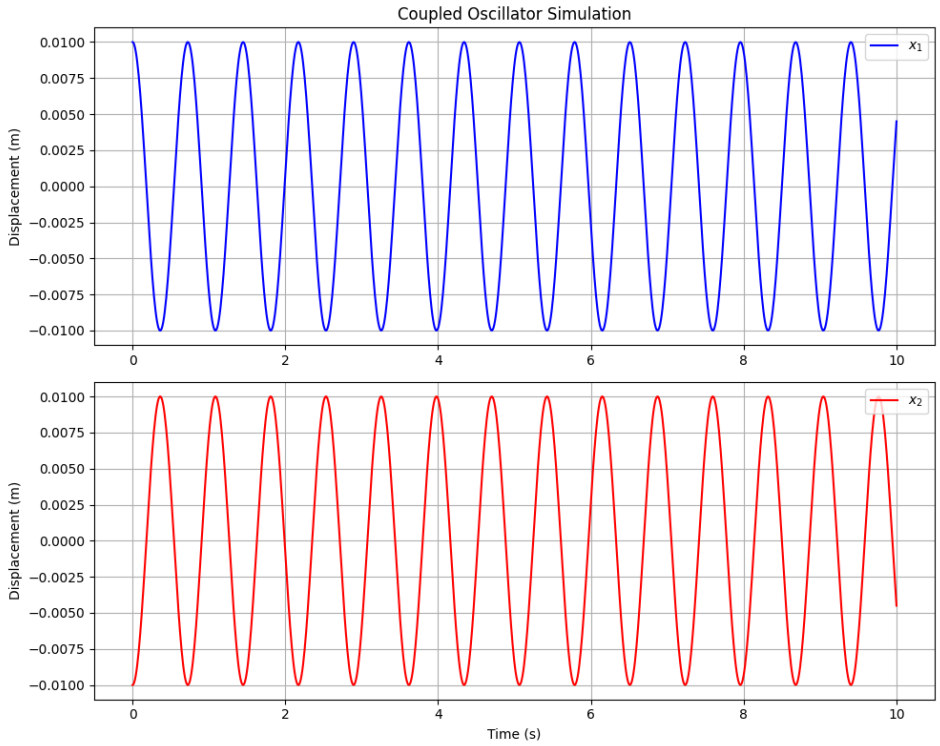
Python

```python
import numpy as np
from scipy.integrate import solve_ivp
import matplotlib.pyplot as plt

# Constants
m = 0.1  # mass in kg
l = 0.15  # length in m
k = 0.5  # spring constant in N/m
g = 9.81  # acceleration due to gravity in m/s^2

# Initial conditions
def coupled_oscillators(name, x1_0 = 0.01, x2_0 = 0.01, v1_0 = 0.0, v2_0 = 0.0):
  '''
  x1_0 = 0.01  # initial position of x1 in m
  x2_0 = 0.01  # initial position of x2 in m
  v1_0 = 0.0  # initial velocity of x1
  v2_0 = 0.0  # initial velocity of x2
  '''

  # System of equations
  def _ode(t, y):
    x1, v1, x2, v2 = y
    dx1dt = v1
    dv1dt = -(g / l) * x1 - (k / m) * (x1 - x2)
    dx2dt = v2
    dv2dt = -(g / l) * x2 - (k / m) * (x2 - x1)
    return [dx1dt, dv1dt, dx2dt, dv2dt]

  # Time span for the simulation
  t_span = (0, 10)  # simulate from t=0 to t=10 seconds
  t_eval = np.linspace(t_span[0], t_span[1], 1000)  # time points to evaluate at

  # Initial state vector
  y0 = [x1_0, v1_0, x2_0, v2_0]

  # Solve the system of ODEs
  solution = solve_ivp(_ode, t_span, y0, t_eval=t_eval)

  # Plot the results on separate subplots
  plt.figure(figsize=(10, 8))

  # Plot for x1
  plt.subplot(211)
  plt.plot(solution.t, solution.y[0], label=r'$x_1$', color='b')
```

```
    plt.ylabel('Displacement (m)')
    plt.title('Coupled Oscillator Simulation')
    plt.legend(loc='upper right')
    plt.grid(True)

    # Plot for x2
    plt.subplot(212, sharex=plt.gca())
    plt.plot(solution.t, solution.y[2], label=r'$x_2$', color='r')
    plt.xlabel('Time (s)')
    plt.ylabel('Displacement (m)')
    plt.legend(loc='upper right')
    plt.grid(True)

    plt.tight_layout()
    plt.savefig(f"img/mechanical-bloch-f1-{name}.png")

coupled_oscillators("1", 0.01, 0.01)
coupled_oscillators("2", 0.01, -0.01)
```

Result





2.2 Discussion

2.2.1 Simulation

User:

Hi model. Please consider the below example file (Latex) describing a working simulation of the Maxwell equation:
/append file:maxwell-sim.tex in
(end of example).
I have the following formulas describing a coupled oscillator:

$$\ddot{x}_1 + \frac{g}{\ell}x_1 + \frac{k}{m}(x_1 - x_2) = 0,$$
$$\ddot{x}_2 + \frac{g}{\ell}x_2 + \frac{k}{m}(x_2 - x_1) = 0$$

Please generate me a code in Python which would simulate these formulas, given $m = 0.1$ kg, $l = 0.15$ m, $k = 0.5$ N/m, At $t = 0$, let both $x_1 = 1$ cm and $x_2 = 1$ cm.

AI:

To simulate the system of coupled oscillators described by the differential equations, we can use numerical integration methods. One common approach is the *Runge-Kutta method*, which is well-suited for

solving ordinary differential equations (ODEs). Here's a Python code example that sets up and solves the system using the `scipy` library's `solve_ivp` function:

Python

```python
import numpy as np
from scipy.integrate import solve_ivp
import matplotlib.pyplot as plt

# Constants
m = 0.1  # mass in kg
l = 0.15  # length in m
k = 0.5  # spring constant in N/m
g = 9.81  # acceleration due to gravity in m/s^2

# Initial conditions
x1_0 = 0.01  # initial position of x1 in m
x2_0 = 0.01  # initial position of x2 in m
v1_0 = 0.0  # initial velocity of x1
v2_0 = 0.0  # initial velocity of x2

# System of equations
def coupled_oscillators(t, y):
  x1, v1, x2, v2 = y
  dx1dt = v1
  dv1dt = -(g / l) * x1 - (k / m) * (x1 - x2)
  dx2dt = v2
  dv2dt = -(g / l) * x2 - (k / m) * (x2 - x1)
  return [dx1dt, dv1dt, dx2dt, dv2dt]

# Time span for the simulation
t_span = (0, 10)  # simulate from t=0 to t=10 seconds
t_eval = np.linspace(t_span[0], t_span[1], 1000)  # time points to evaluate at

# Initial state vector
y0 = [x1_0, v1_0, x2_0, v2_0]

# Solve the system of ODEs
solution = solve_ivp(coupled_oscillators, t_span, y0, t_eval=t_eval)

# Plot the results on separate subplots
plt.figure(figsize=(10, 8))

# Plot for x1
plt.subplot(211)
plt.plot(solution.t, solution.y[0], label=r'$x_1$', color='b')
plt.ylabel('Displacement (m)')
plt.title('Coupled Oscillator Simulation')
plt.legend(loc='upper right')
plt.grid(True)

# Plot for x2
plt.subplot(212, sharex=plt.gca())
plt.plot(solution.t, solution.y[2], label=r'$x_2$', color='r')
plt.xlabel('Time (s)')
plt.ylabel('Displacement (m)')
plt.legend(loc='upper right')
plt.grid(True)
```

```
plt.tight_layout()
plt.show()
```

The code sets up the system of differential equations for the coupled oscillators based on the provided formulas. It defines initial conditions for x_1 and x_2 as 1 cm = 0.01 m, and uses the `solve_ivp` function from `scipy.integrate` to perform the integration over the specified time span. The results are then plotted using `matplotlib` to visualize the displacement over time for both oscillators.

2.2.2 Runge-Kutta

User:

Please tell me more about Runge-Kutta method. What kind of DE can it solve?

AI:

The Runge-Kutta methods are a family of iterative methods used for approximating solutions to ordinary differential equations (ODEs). They are known for their accuracy and efficiency, making them a popular choice for solving a wide range of ODEs, particularly when analytical solutions are challenging or impossible to obtain.

Here are some key aspects of the Runge-Kutta methods:

- **Types of Equations:**
  - Runge-Kutta methods are primarily used for first-order ODEs of the form:

    $$\frac{dy}{dt} = f(t, y)$$

    where y is the dependent variable, t is the independent variable, and f is a function that describes the system.
  - Higher-order ODEs can be solved by converting them into a system of first-order ODEs. For example, a second-order ODE can be rewritten using two first-order ODEs by introducing auxiliary variables for each derivative.
- **The Classical Fourth-Order Runge-Kutta Method (RK4):**
  - The RK4 method is a popular version that provides a good balance between accuracy and computational cost. It estimates the solution by taking the weighted average of slopes (derivatives) at several points within the integration step.
  - The RK4 algorithm involves four intermediate calculations, known as *stages*, per time step to approximate the next value:

$$\begin{aligned}
k_1 &= f(t_n, y_n), \\
k_2 &= f\left(t_n + \frac{\Delta t}{2}, y_n + \frac{k_1 \Delta t}{2}\right), \\
k_3 &= f\left(t_n + \frac{\Delta t}{2}, y_n + \frac{k_2 \Delta t}{2}\right), \\
k_4 &= f(t_n + \Delta t, y_n + k_3 \Delta t),
\end{aligned}$$

- The next value of y is then found by:

$$y_{n+1} = y_n + \frac{\Delta t}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

- **Applications:**
  - Runge-Kutta methods can be used to solve a vast range of problems, including systems modeling physical phenomena (e.g., mechanics, orbital dynamics), biological processes, electrical circuits, and any situation well-modeled by ODEs.
  - They can handle various initial value problems and are appropriate for stiff and non-stiff ODEs when carefully chosen. However, for very stiff equations, specialized methods (like implicit Runge-Kutta methods) might be more suitable.
- **Advantages and Limitations:**
  - Runge-Kutta methods are straightforward to implement, versatile, and capable of high precision.
  - They are computationally intensive compared to simpler methods like Euler's method, but generally offer better stability and accuracy.
  - They require careful step-size control; adaptive step-size versions of the Runge-Kutta methods can be used to achieve better efficiency and accuracy.

The Runge-Kutta methods, with RK4 being the most widely implemented, are robust tools for numerically solving a broad class of ODEs encountered in scientific computing, engineering, and physics.

2.2.3 Runge-Kutta vs FDTD

User:

Can you compare Runge-Kutta with FDTD method?

AI:

Certainly! Both the Runge-Kutta and Finite-Difference Time-Domain (FDTD) methods are numerical techniques used for solving differential equations, but they are employed in different contexts and have distinct characteristics. Let's compare them:

- **Purpose and Application:**
  - **Runge-Kutta (RK) Methods:** - Primarily designed for solving ordinary differential equations (ODEs). - Widely used in a variety of fields, such as engineering, physics, and other sciences, for problems involving time-dependent systems or dynamics. - A versatile choice for systems where the equations involve one independent variable, often time.

  - **Finite-Difference Time-Domain (FDTD) Method:** - Specifically developed for solving Maxwell's equations in the time-domain to model electromagnetic wave propagation. - Commonly applied in computational electromagnetics for simulating fields around antennas, waveguides, and other RF/microwave structures. - Suitable for partial differential equations (PDEs) involving both spatial and time dimensions.

- **Algorithm and Technique:**

  - **Runge-Kutta Methods:** - Use multiple stages (e.g., 4 stages in RK4) to improve accuracy by estimating the solution's slope at various points within each time step. - Considered explicit methods; they work step-by-step using initial conditions without needing to solve simultaneous equations at each time step.
  - **FDTD Method:** - Based on discretizing both space and time using finite differences, approximating derivatives with differences. - Applies both explicit and sometimes implicit techniques to update field values in a grid iteratively. - Used extensively in grid-based simulations of wave interactions where spatial-temporal accuracy is essential.

- **Strengths and Use Cases:**

  - **Runge-Kutta Methods:** - High precision for well-posed initial value problems in ODEs. - Preferred for non-stiff and moderately stiff systems with complex dynamics. - Adaptive step-size versions allow efficient computation.
  - **FDTD Method:** - Excellent for capturing wave phenomena and field interactions in heterogeneous media. - Direct simulation of wave reflections, diffraction, interference, and scattering. - Highly parallelizable; often implemented in parallel computing frameworks.

- **Limitations:**

  - **Runge-Kutta Methods:** - Only suitable for ordinary differential equations (one independent variable). - Can be computationally intensive for very stiff systems.
  - **FDTD Method:** - Computationally demanding, requiring fine spatial and temporal discretization to maintain accuracy. - Requires careful handling of boundary conditions to prevent artificial reflections.

In essence, while both Runge-Kutta and FDTD methods aim to numerically solve differential equations, they cater to different types of problems. The Runge-Kutta method is a general-purpose tool for ODEs, whereas FDTD is specialized for simulating electromagnetic fields and wave interactions governed by Maxwell's equations.

2.2.4 ODE

User:

OK, now please define ordinary DE. What is dependant variable? Why is it different from a function?

AI:

An ordinary differential equation (ODE) is a type of differential equation involving functions of a single

independent variable and their derivatives. ODEs describe the rate of change of a dependent variable with respect to an independent variable. Here is a more detailed explanation:

- **Definition of ODE:**
  - An ODE can be written in its general form as:

$$F\left(t, y, \frac{dy}{dt}, \frac{d^2y}{dt^2}, \ldots, \frac{d^ny}{dt^n}\right) = 0$$

    where y is a dependent variable, t is the independent variable, and F is a function representing the relationship between these variables and their derivatives.
  - The order of an ODE is determined by the highest derivative of the dependent variable present in the equation. For example, a first-order ODE involves only the first derivative $\frac{dy}{dt}$.
  - ODEs are classified into linear and nonlinear equations based on the degree of the dependent variable and its derivatives. Linear ODEs have the dependent variable and its derivatives to the power of one, without multiplication between them.
- **Dependent Variable:**
  - The dependent variable (y in our example) is the quantity whose variations we are interested in studying. It is typically a function of the independent variable.
  - In the context of an ODE, the dependent variable represents the unknown whose behavior is described by the differential equation. It changes in response to changes in the independent variable.
  - The solution to an ODE is a function $y(t)$ describing how the dependent variable evolves over the domain of the independent variable.
- **Difference from a Function:**
  - While the dependent variable is a specific variable being solved for in an ODE, a function is a broader mathematical concept representing a relationship between variables, typically defined by an explicit formula or rule.
  - In an ODE, $y(t)$ is the function that serves as the solution, expressing the dependent variable in terms of the independent variable. It describes the behavior or state of the dependent variable over time or space.
  - The outcome of solving an ODE is the function itself, which reveals how the dependent variable changes, providing insights into the underlying dynamic system.

In summary, ODEs play a crucial role in modeling a wide array of real-world phenomena where a single independent variable influences the behavior of another variable, such as time-dependent processes in physics, engineering, and beyond.

3 Following the paper

(2014, Frimmer and Novotny) "The classical Bloch equations" [1].
The main motion equations are:

$$m\frac{d^2x_A}{dt^2} + m\gamma\frac{dx_A}{dt} + (k + \kappa - \Delta k(t))\, x_A - \kappa x_B = F(t)$$
$$m\frac{d^2x_B}{dt^2} + m\gamma\frac{dx_B}{dt} + (k + \kappa + \Delta k(t))\, x_B - \kappa x_A = 0$$

Dividing by m.

$$\frac{d^2x_A}{dt^2} + \gamma\frac{dx_A}{dt} + \left(\frac{k+\kappa}{m} - \frac{\Delta k(t)}{m}\right) x_A - \frac{\kappa}{m}x_B = \frac{1}{m}F(t)$$
$$\frac{d^2x_B}{dt^2} + \gamma\frac{dx_B}{dt} + \left(\frac{k+\kappa}{m} + \frac{\Delta k(t)}{m}\right) x_B - \frac{\kappa}{m}x_A = 0$$

Introducing Ω frequencies:

$$\Omega_0^2 = [k+\kappa]/m$$

$$\Omega_d^2 = \Delta k/m$$

$$\Omega_c^2 = \kappa/m$$

becomes

$$\left(\tfrac{d^2}{dt^2} + \gamma\tfrac{d}{dt} + \Omega_0^2\right)\begin{pmatrix}x_A\\x_B\end{pmatrix} + \begin{pmatrix}-\Omega_d^2 & -\Omega_c^2\\ -\Omega_c^2 & \Omega_d^2\end{pmatrix}\begin{pmatrix}x_A\\x_B\end{pmatrix} = \begin{pmatrix}F(t)\\0\end{pmatrix}$$

User:

Please rewrite the below two equation into the matrix form. I'd like to be like

`(...)(x_A ; x_B) + (...) (x_A; x_B) = (f(t) ; 0)`.

$$\frac{d^2x_A}{dt^2} + \gamma\frac{dx_A}{dt} + \left(\frac{k+\kappa}{m} - \frac{\Delta k(t)}{m}\right) x_A - \frac{k}{m}x_B = \frac{1}{m}F(t)$$
$$\frac{d^2x_B}{dt^2} + \gamma\frac{dx_B}{dt} + \left(\frac{k+\kappa}{m} + \frac{\Delta k(t)}{m}\right) x_B - \frac{k}{m}x_A = 0$$

Introducing Ω frequencies:

$$\Omega_0^2 = [k+\kappa]/m$$

$$\Omega_d^2 = \Delta k/m$$

$$\Omega_c^2 = \kappa/m$$

AI:

To rewrite the given equations in matrix form, we'll utilize the newly introduced frequencies Ω_0, Ω_d, and Ω_c. We then represent the system using matrix operations on a vector composed of x_A and x_B. The two equations provided are:

$$\frac{d^2x_A}{dt^2} + \gamma\frac{dx_A}{dt} + \left(\frac{k+\kappa}{m} - \frac{\Delta k(t)}{m}\right)x_A - \frac{k}{m}x_B = \frac{1}{m}F(t)$$

$$\frac{d^2x_B}{dt^2} + \gamma\frac{dx_B}{dt} + \left(\frac{k+\kappa}{m} + \frac{\Delta k(t)}{m}\right)x_B - \frac{k}{m}x_A = 0$$

Using the new frequency parameters, the equations become:

$$\frac{d^2x_A}{dt^2} + \gamma\frac{dx_A}{dt} + \left(\Omega_0^2 - \Omega_d^2\right)x_A - \frac{k}{m}x_B = \frac{1}{m}F(t)$$

$$\frac{d^2x_B}{dt^2} + \gamma\frac{dx_B}{dt} + \left(\Omega_0^2 + \Omega_d^2\right)x_B - \frac{k}{m}x_A = 0$$

To express these in a matrix form:

$$\begin{pmatrix} \frac{d^2}{dt^2} + \gamma\frac{d}{dt} + (\Omega_0^2 - \Omega_d^2) & -\frac{k}{m} \\ -\frac{k}{m} & \frac{d^2}{dt^2} + \gamma\frac{d}{dt} + (\Omega_0^2 + \Omega_d^2) \end{pmatrix} \begin{pmatrix} x_A \\ x_B \end{pmatrix} = \begin{pmatrix} \frac{1}{m}F(t) \\ 0 \end{pmatrix}$$

This representation condenses the system of differential equations into a single matrix equation, allowing easier manipulation and understanding of the coupled dynamics.

References

[1] Martin Frimmer and Lukas Novotny. "The classical Bloch equations". In: *American Journal of Physics* 82.10 (Oct. 2014), pp. 947–954. ISSN: 1943-2909. DOI: 10.1119/1.4878621. URL: http://dx.doi.org/10.1119/1.4878621.

[2] W.F. Smith. *Waves and Oscillations: A Prelude to Quantum Mechanics*. Oxford University Press, 2010. ISBN: 9780199742127. URL: https://api.semanticscholar.org/CorpusID:118019131.