Lecture 4: Differential Equations (II)

(Inspired from slides by Uriel Morzan)

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18. Oct. 2023

Introduction

Last lecture:

- Euler & midpoint method for a system of 1st order ODEs (pendulum).

Today:

- Euler & Verlet method for a 1st order ODE of a complex matrix (qubit).

Brief Intro to the State of a Qubit

The state of a "Qubit" (short for quantum bit = two level system) can be described with a density matrix ρ. For a pure state $\rho = |\psi\rangle\langle\psi|$. After choosing an orthonormal basis set, e.g. $\{|g\rangle, |e\rangle\}$ the density matrix can be expressed as a 2x2 complex matrix

$$\rho = \begin{pmatrix} \langle g|\rho|g\rangle & \langle g|\rho|e\rangle \\ \langle e|\rho|g\rangle & \langle e|\rho|e\rangle \end{pmatrix}.$$

With a density matrix we can describe both:

- **quantum superposition** For example, the equal quantum superposition of ground and excited state $|+\rangle = \frac{1}{\sqrt{2}}(|g\rangle + |e\rangle)$ is

$$\rho_+ = |+\rangle\langle+| = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix}.$$

- **stochastic mixtures** For example, the stochastic mixture of ground and excited state is

$$\rho_M = \frac{1}{2}|g\rangle\langle g| + \frac{1}{2}|e\rangle\langle e| = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}.$$

Brief Intro to the State of a Qubit

Not any complex 2x2 matrix is a valid physical state of a qubit:

1. *positive*: all eigenvalues of ρ must be real and non-negative.
2. *hermitian*: $\rho \overset{!}{=} \rho^\dagger$.
3. *trace class*: $\mathrm{tr}\,(\rho) \overset{!}{=} 1$

Also, a state is pure (which means it is not a stochastic mixture) $\Leftrightarrow \mathrm{tr}(\rho^2) = 1$.

The density matrix of a qubit in the ground state in FORTRAN:

```
complex, dimension(2,2) :: rho
rho(1,1)=(1.00,0.00)
rho(1,2)=(0.00,0.00)
rho(2,1)=(0.00,0.00)
rho(2,2)=(0.00,0.00)
```

$$\rho = |g\rangle\langle g| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Evolution of a Qubit: Von Neumann Equation

The von Neumann equation is the Schrödinger equation formulated for density matrices:

$$\frac{\partial \rho}{\partial t} = -i\left(H \cdot \rho - \rho \cdot H\right)$$

```
drho_dt = (0.0,-1.0) * (matmul(H,rho) - matmul(rho,H))
```

H is the Hamiltonian divided by $\hbar$ and a 2x2 complex matrix, for example:

```
complex, dimension(2,2) :: H
H(1,1) = (0.0, 0.0)
H(1,2) = (0.7, 0.2)
H(2,1) = (0.7, -0.2)
H(2,2) = (1.0, 0.0)
```

$$H = \begin{pmatrix} 0.0 & 0.7 + 0.2i \\ 0.7 - 0.2i & 1.0 \end{pmatrix}$$

Verlet Method

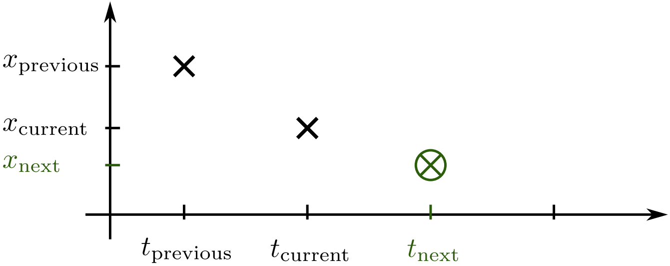
The von Neumann equation is a 1st order differential equation of the form $\frac{\mathrm{d}x}{\mathrm{d}t} = f(t, x)$. We already know the Euler and the midpoint method to solve such a differential equation.

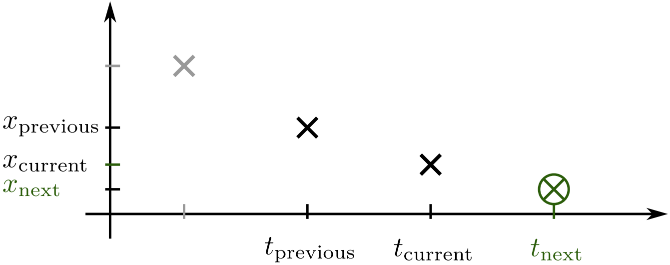
Let's add another method to our toolbox! Consider the two Taylor expansions:

$$\rho(t + \Delta t) = \rho(t) + \frac{\partial \rho}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 \rho}{\partial t^2}\Delta t^2 + \mathcal{O}(\Delta t^3)$$
$$\rho(t - \Delta t) = \rho(t) - \frac{\partial \rho}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 \rho}{\partial t^2}\Delta t^2 + \mathcal{O}(\Delta t^3)$$

$$\Rightarrow \quad x(t + \Delta t) \quad \approx \quad x(t - \Delta t) + 2 \cdot f(t, x(t)) \cdot \Delta t$$

Verlet Method Algorithm





Verlet Method Algorithm

Algorithm: Verlet Method

Input: function $f(t,x)$, initial values t_0, x_0, step size Δt, and number of steps N

1. set $x_{\text{previous}} := x_0$
2. compute x_{current} for $t_{\text{current}} := t_0 + \Delta t$ with another method (e.g. midpoint method)
3. repeat $N-1$ times:
   - set $fx_{\text{current}} := f(t_{\text{current}}, x_{\text{current}})$
   - set $x_{\text{next}} := x_{\text{previous}} + 2 \cdot fx_{\text{current}} \cdot \Delta t$
   - set $t_{\text{current}} := t_{\text{current}} + \Delta t$
   - set $x_{\text{previous}} := x_{\text{current}}$
   - set $x_{\text{current}} := x_{\text{next}}$

Output: the sequence of t and x approximating the solution of $\frac{\mathrm{d}x}{\mathrm{d}t} = f(t,x)$.

Assignment 11

Write a program that solves the equation of motion for the density matrix of a qubit $\rho(t)$ using the Euler and the Verlet method:

- Create a separate subroutine `drho_dt(t,rho,H,res)`
- Create separate subroutines `euler(t0, rho0, H, dt, N)` and `verlet(t0, rho0, H, dt, N)`
- The subroutines should each create a file (`euler.txt` and `verlet.txt`) with result of the computations in three columns: t, $\langle g|\rho(t)|g\rangle$, $\langle e|\rho(t)|e\rangle$.
- Use as initial conditions $t_0 = 0.0$, $\rho_0 = |g\rangle\langle g|$ and the Hamiltonian from slide 5.
- Plot the results for the Euler method and Verlet method with $\Delta t = 0.05$ and $N = 300$.
- What is unphysical about the Euler result?
- Submit the two graphs and your code as `<surname>-assignment-11.f90` to gfux@ictp.it before the next lesson.

Suggested Starting Point for Assignment 11

```fortran
program qubit
  ! ... DECLARE THE INITIAL CONDITIONS AND CALL euler(...)

contains

  subroutine euler(t0,rho0,H,dt,N)
    ! ... IMPLEMENT THE EULER METHOD
  end subroutine euler

  subroutine drho_dt(t,rho,H,res)
    real, intent(in) :: t
    complex, dimension(:,:), intent(in) :: rho, H
    complex, dimension(:,:), intent(out) :: res ! result
    res = ! ... COMPLETE THIS LINE
  end subroutine drho_dt

end program qubit
```