Computational Physics

Lorentz model

final report

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Problem to solve

If we applied electric field to the dielectric material, the electric charges in dielectric material will slightly move away from their average equilibrium positions, which causes dielectric polarization. And in our final project, we want to know how long the charges will move away from the average equilibrium positions. By Lorentz model we have:

$$\frac{d^2x}{dt^2}+\gamma\frac{dx}{dt}+\omega_0^2x=\frac{F(t)}{m} \tag{1}$$

where $F(t)$ is the electric force, and can be written as:

$$F(t)=-eE(t) \tag{2}$$

by solving the secondary ordinary differential equation, we can obtain the solution of $x(t)$.

By Maxwell's equation, we can conclude that the refractive index of the dielectric material as:

$$n\approx\sqrt{\varepsilon_1} \tag{3}$$

and ε_1 in (3) is equal to:

$$\varepsilon_1=1+\chi_{bg}+\frac{Ne^2}{\varepsilon_0 m}\frac{(\omega_0^2-\omega^2)}{(\omega_0^2-\omega^2)^2+(\gamma\omega)^2} \tag{4}$$

We can fit the refractive index curve of the material and obtain the value of χ_{bg} 、 γ, thus we can use these to solve the ODE numerically.

Problem 1:

By fitting the analytical formalism of refractive index in the Lorentz model, find the parameters, $\chi_{bg} = ?, \gamma = ?$, best fitted to the measurement.

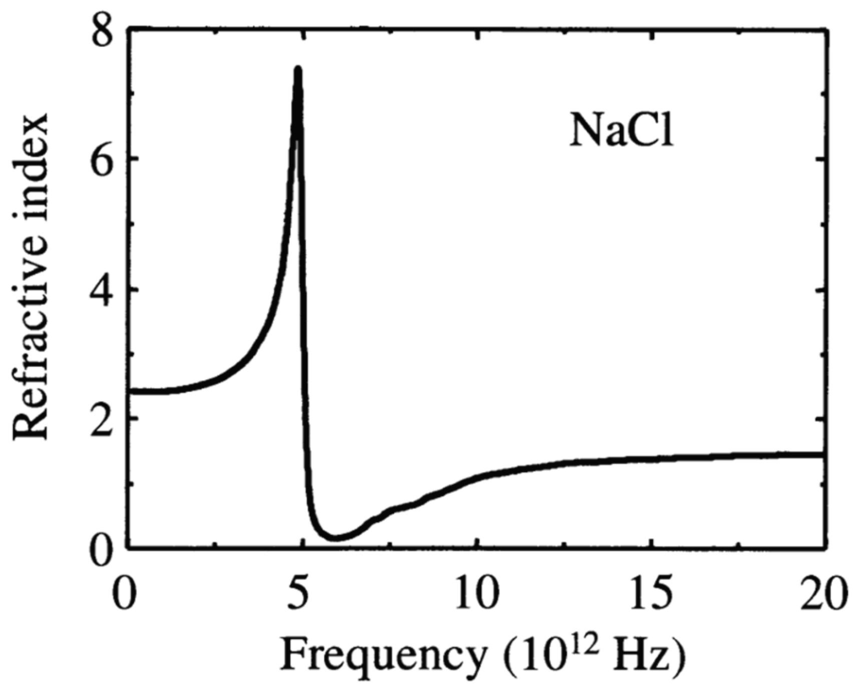


Fig. 2.13 Infrared refractive index of NaCl. After [1].

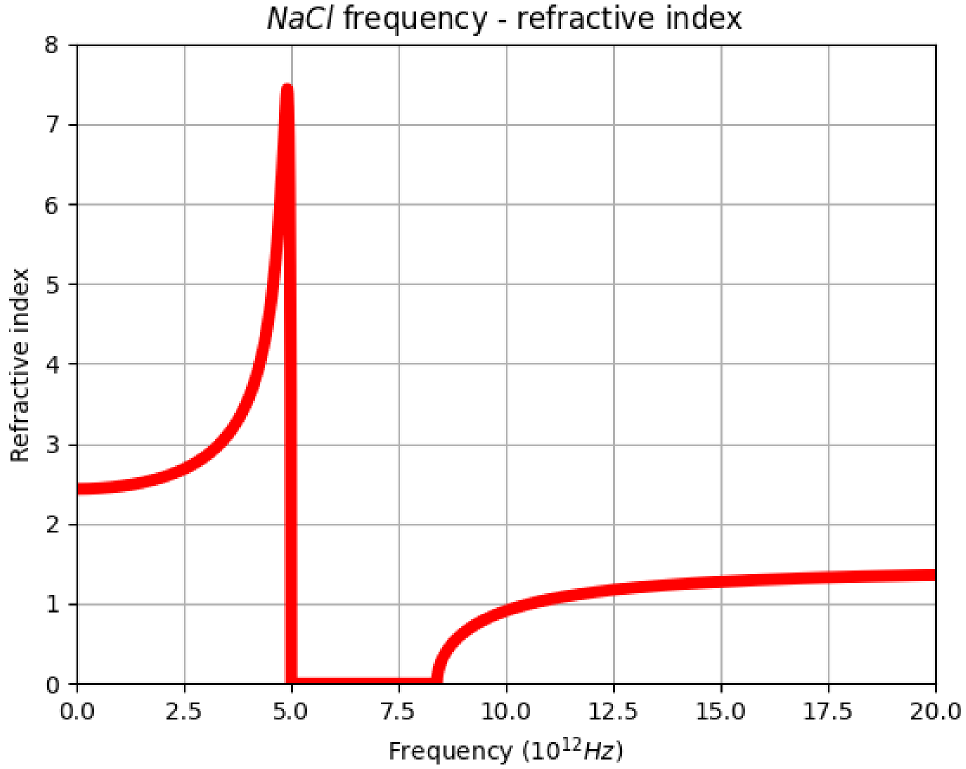
Solution:

There is no strategy in this problem, just remind the unit of the physical quantities! By (3) and (4), we can use the horizontal asymptote line of the graph when $\omega \to \infty$ to calculate the value of χ_{bg}

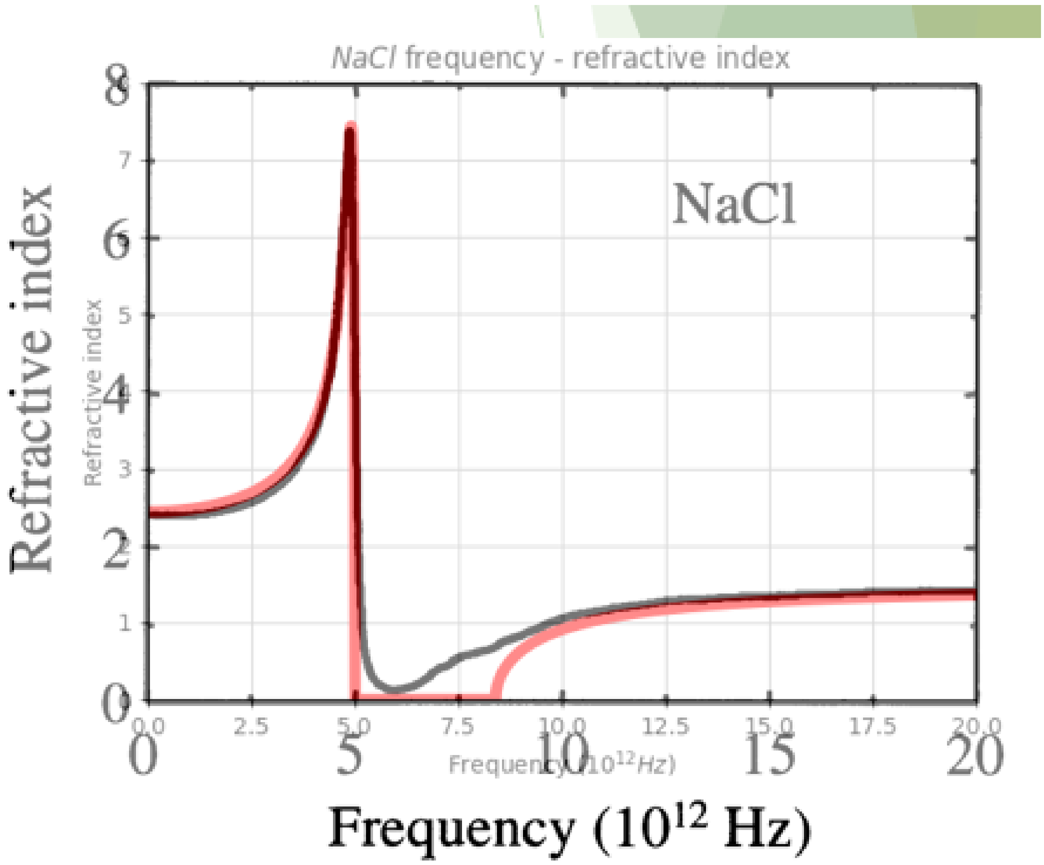
$$\lim_{\omega\to\infty} n = \sqrt{\varepsilon_1} = \sqrt{1+\chi_{bg} + \frac{Ne^2}{\varepsilon_0 m} \frac{\left(\omega_0^2 - \omega^2\right)}{\left(\omega_0^2 - \omega^2\right)^2 + \left(\gamma\omega\right)^2}} = \sqrt{1+\chi_{bg}} \approx 1.45 \Rightarrow \chi_{bg} = 1.10$$

and I use $\gamma = 1.15 \cdot 10^{12} \left(rad / s\right)$ to best fit the graph

Result:



Overlap with the original graph:



Parameter setting:

χ_{bg}	1.10
m	$2.3\cdot10^{-26}\left(kg\right)$
ω_0	$2\pi\cdot5\cdot10^{12}\left(rad/s\right)$
N	$3\cdot10^{28}\left(m^{-3}\right)$
γ	$1.15\cdot10^{12}\left(rad/s\right)$
e	$1.6\cdot10^{-19}\left(C\right)$
ε_0	$8.854\cdot10^{-12}\left(Farad/m\right)$

```
#parameter of NaCl:
χ_bg=1.1
m=2.3*(10**(-26))             #(kg)
omega_0=5*2*np.pi*(10**12)    #(rad/s)
N=3*(10**28)                  #(m^-3)
γ=1.15*(10**12)              #(rad/s)
e=1.6*(10**(-19))             #(C)
ε_0=8.854*(10**-12)           #(Farad/m)
```

Function to calculate the refractive index:

```
def refractive_index(omega):
    ε_1=1+χ_bg+k*((omega_0**2)-(omega**2))/((((omega_0**2)-
(omega**2))**2)+((γ*omega)**2))
    if ε_1<0:
        ε_1=0
    return np.sqrt(ε_1)
```

Note that we use the formula in (3) and (4), and that's a simplify formula. That's the reason why we didn't fit the graph precisely on the frequency on the range of $5\sim8(10^{12}\,Hz)$

If we want to fit this range precisely, then we need to consider the more general formula:

$$\tilde{\varepsilon}_r = \varepsilon_1 + i\varepsilon_2 \in \mathbb{C} \tag{5}$$

And since:

$$\tilde{n} = \sqrt{\tilde{\varepsilon}_r} = n + ik \tag{6}$$

We can solve n 、 k in terms of ε_1 and ε_2:

$$n = \frac{\sqrt{\left[\varepsilon_1 + \sqrt{\left(\varepsilon_1^2 + \varepsilon_2^2\right)}\right]}}{\sqrt{2}}, k = \frac{\sqrt{\left[-\varepsilon_1 + \sqrt{\left(\varepsilon_1^2 + \varepsilon_2^2\right)}\right]}}{\sqrt{2}} \tag{7}$$

As $|\varepsilon_1| \gg |\varepsilon_2|$ at most time, we can simplify $\tilde{n}$ as:

$$\tilde{n} \approx \sqrt{\varepsilon_1} \tag{8}$$

However, in our fitting problem, it seems that $|\varepsilon_1| \gg |\varepsilon_2|$ didn't occur when frequency on the range of $5 \sim 8(10^{12} Hz)$. Thus, I set $\varepsilon_1 = 0$ to avoid the warning of the negative number during the root square procedure. Except for the range of $5 \sim 8(10^{12} Hz)$, I fitted the curve exactly!

In this problem, I learn how to fit the curve. And I think it is definitely an important skill for me. Use the initial point and choose some vertical or horizontal asymptotes to calculate the scale of the parameter. And with the help of computer, we can easily obtain the best-fitted parameter in the formula.

Problem 2:

Present the dynamical electron displacement, $x(t)$, as a function of time, t, under the following conditions:

$(a)\,\omega \ll \omega_0$

$(b)\,\omega \lesssim \omega_0$

$(c)\,\omega \gtrsim \omega_0$

$(d)\,\omega \gg \omega_0$

Solution:

In this problem, we are asked to solve the equation in (1) and exert a time-dependent force in different ω to see the outcome of $x(t)$.

As we had learned in class, I use Runge-Kutta method to numerical solved the secondary ordinary differential equation:

$$\frac{d^2x}{dt^2}+\gamma\frac{dx}{dt}+\omega_0^2x=\frac{F(t)}{m}$$

First, we rewrite the equation into coupled ODE:

$$\begin{cases}\dfrac{dx}{dt}=v\\[2ex] \dfrac{d^2x}{dt^2}=\dfrac{dv}{dt}=\dfrac{F(t)}{m}-\gamma v-\omega_0^2x\end{cases}\tag{10}$$

And we defined:

$$y_1=x,y_2=v\tag{11}$$

Substitute (11) into (10):

$$\begin{cases} \dfrac{dy_1}{dt} = y_2 \equiv g_1(y_2) \\ \dfrac{dy_2}{dt} = \dfrac{F(t)}{m} - \gamma y_2 - \omega_0^2 y_1 \equiv g_2(y_1, y_2, F(t)) \end{cases} \tag{12}$$

By Runge-Kutta method to calculate the value of y_1, y_2:

$$\begin{cases} y_{1,i+1} \approx y_{1,i} + h\left(\dfrac{k_1}{2} + \dfrac{k_2}{2}\right) \\ k_1 \equiv g_1(y_{2,i}) \\ k_2 \equiv g_1(y_{2,i} + hq_1) \end{cases} \begin{cases} y_{2,i+1} \approx y_{2,i} + h\left(\dfrac{q_1}{2} + \dfrac{q_2}{2}\right) \\ q_1 \equiv g_2(y_{1,i}, y_{2,i}) \\ q_2 \equiv g_2(y_{1,i} + hk_1, y_{2,i} + hq_1) \end{cases} \tag{13}$$

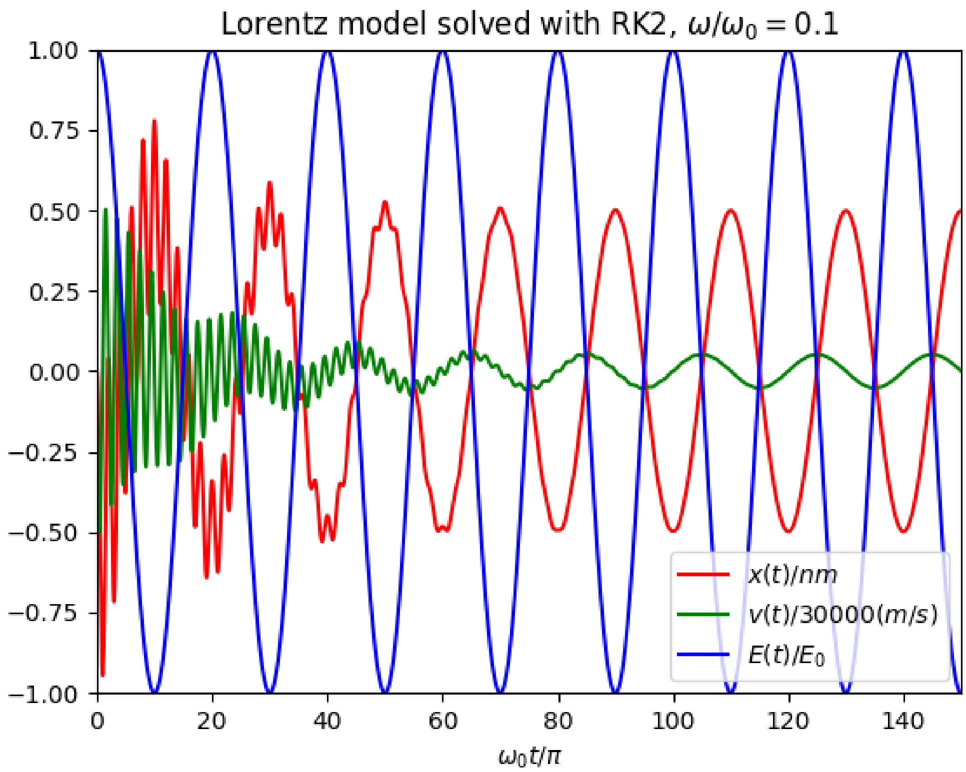
Runge-Kutta method in python code:

```python
def g1(y2):
    return (y2)

def g2(y1,y2,ti):
    F=-1*e*E_0*np.cos(omega*ti)
    return (F/m)-(γ*y2)-((omega_0**2)*y1)

#calculate the value of the next moment by RK2 method
def y_rk2(y1,y2,ti):#with (w1,w2,alpha,beta) = (0.5,0.5,1,1)
    k1=g1(y2)
    q1=g2(y1,y2,ti)
    k2=g1(y2+h*q1)
    q2=g2(y1+h*k1,y2+h*q1,ti+h)
    y1_prime=y1+h*(0.5*k1+0.5*k2)
    y2_prime=y2+h*(0.5*q1+0.5*q2)
    return y1_prime,y2_prime
```

Case $(a)\omega \ll \omega_0$:

choose

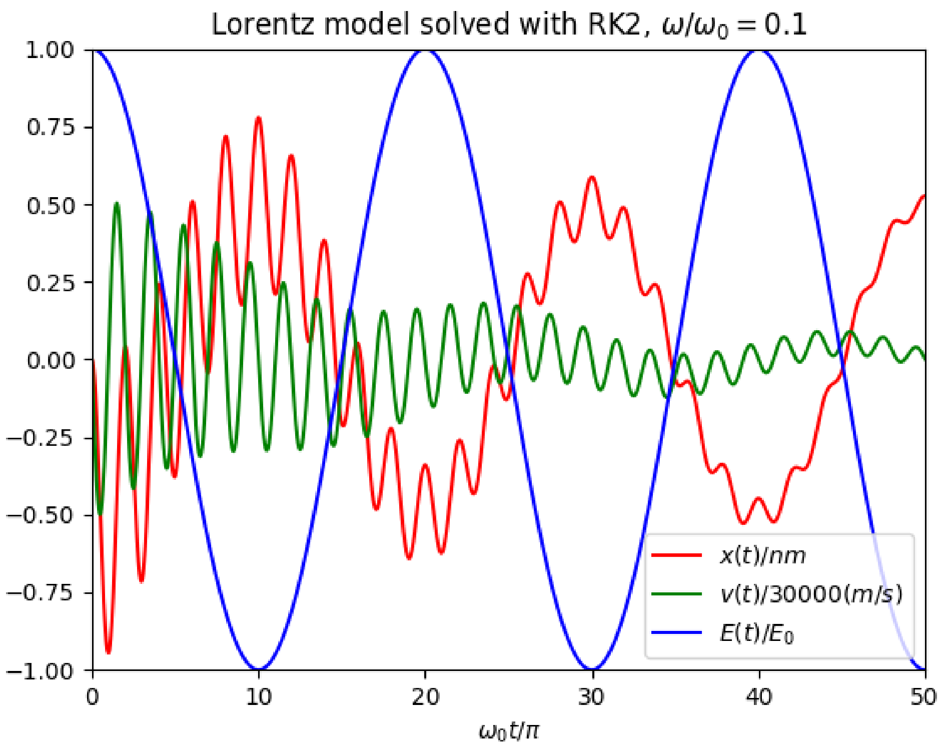
$\omega = 0.1\omega_0 \left(rad / s\right)$ and $E = E_0 \cos\left(\omega t\right)$ & $E_0 = 70 \cdot 10^9 \left(V / m\right)$



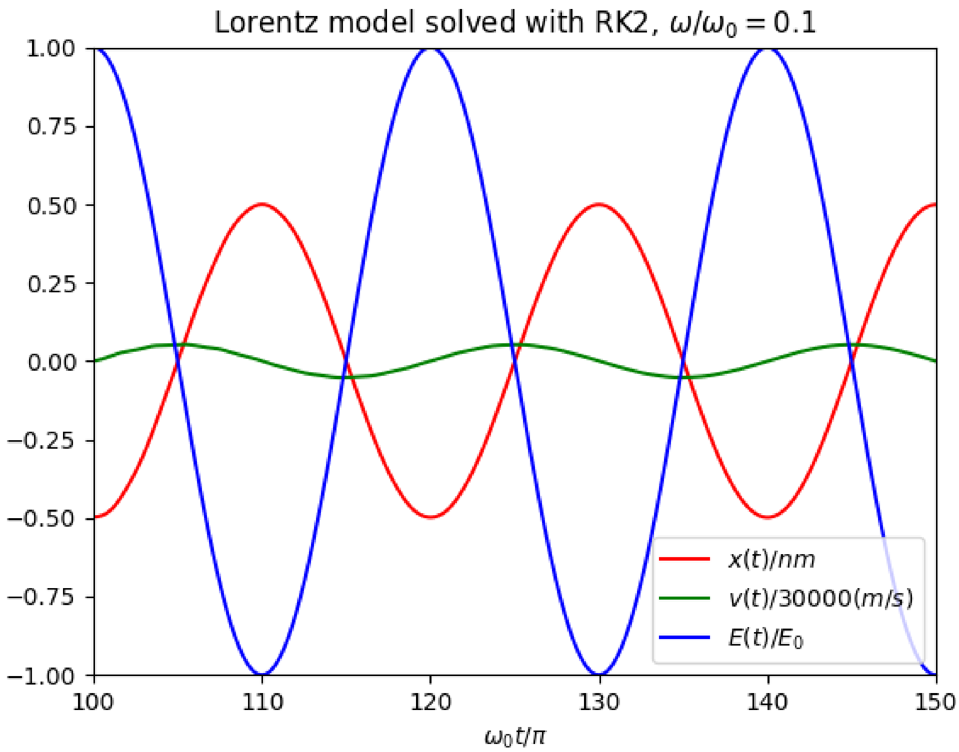
From the graph, we can observe the process from the transient response to the steady-state response, which means after a while, the oscillation will totally contribute by the force we exerted by applying the time-dependent electric field. And the amplitude of $x(t), v(t)$ are both decreasing until they reach the steady-state.

And now I will zoom in some graph in the next page which can be observed the transient state and the steady-state more easily.

Transient response:



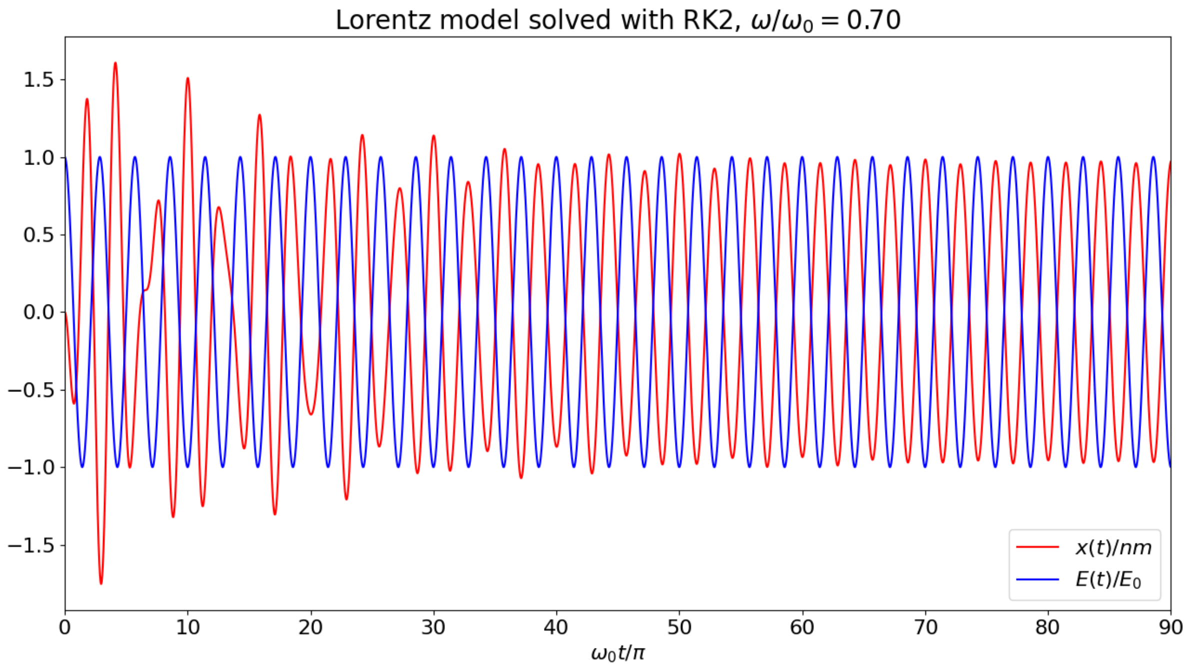
Steady-state response:



Case $(b)\,\omega \lesssim \omega_0$:

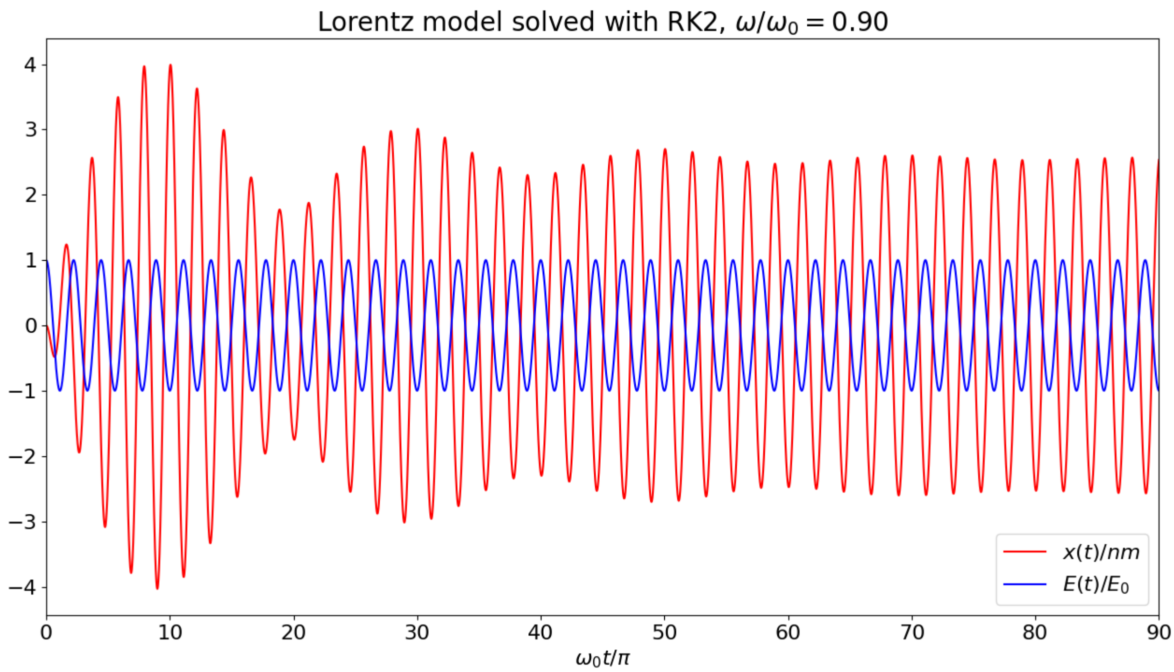
choose

$$\omega = 0.7\omega_0\left(rad/s\right) \text{ and } E = E_0\cos\left(\omega t\right) \;\&\; E_0 = 70\cdot 10^9\left(V/m\right)$$



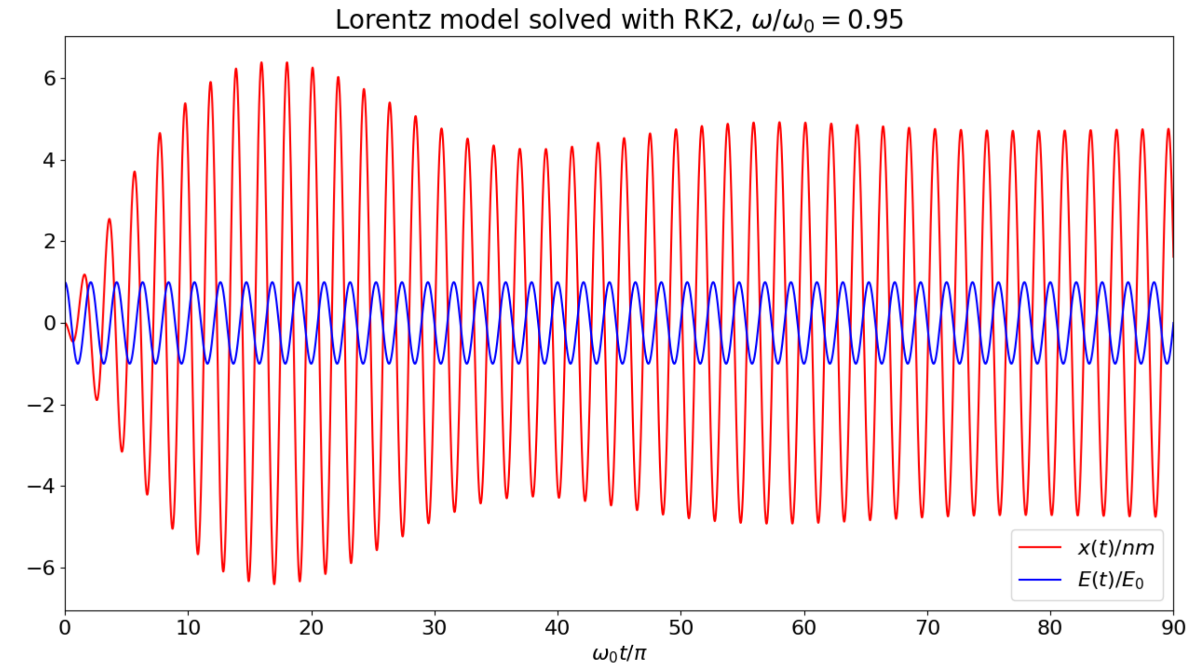
choose

$$\omega = 0.9\omega_0\left(rad/s\right) \text{ and } E = E_0\cos\left(\omega t\right) \;\&\; E_0 = 70\cdot 10^9\left(V/m\right)$$



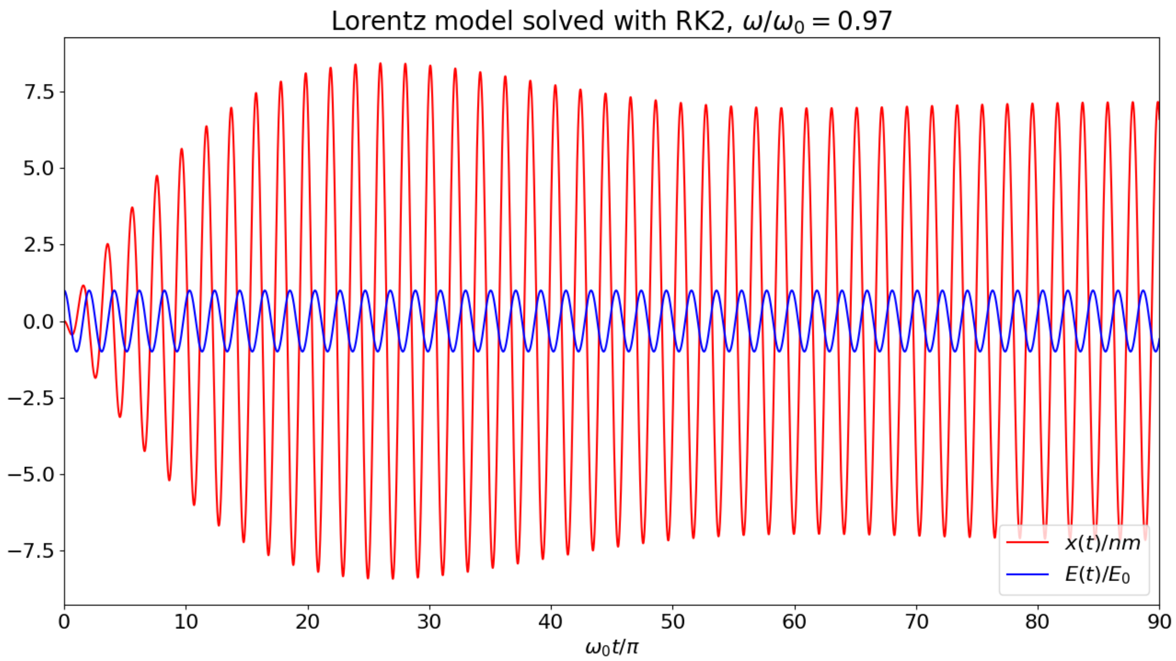
choose

$$\omega = 0.95\omega_0 \left(rad / s\right) \text{ and } E = E_0 \cos\left(\omega t\right) \;\&\, E_0 = 70 \cdot 10^9 \left(V / m\right)$$



choose

$$\omega = 0.97\omega_0 \left(rad / s\right) \text{ and } E = E_0 \cos\left(\omega t\right) \;\&\, E_0 = 70 \cdot 10^9 \left(V / m\right)$$

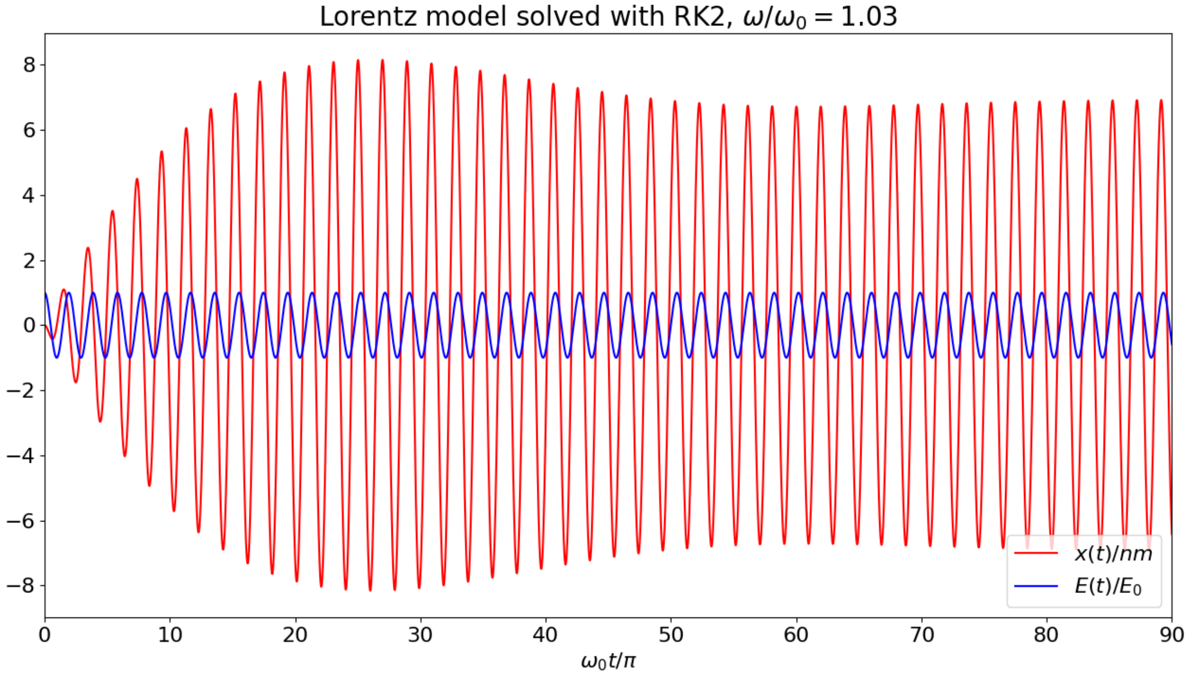


Compare with case a, we can figure out that as the value of ω/ω_0 increase before 1, the amplitude of the solution increases too, and it will need more time to reach the steady state.

Case $(c)\omega \gtrsim \omega_0$:

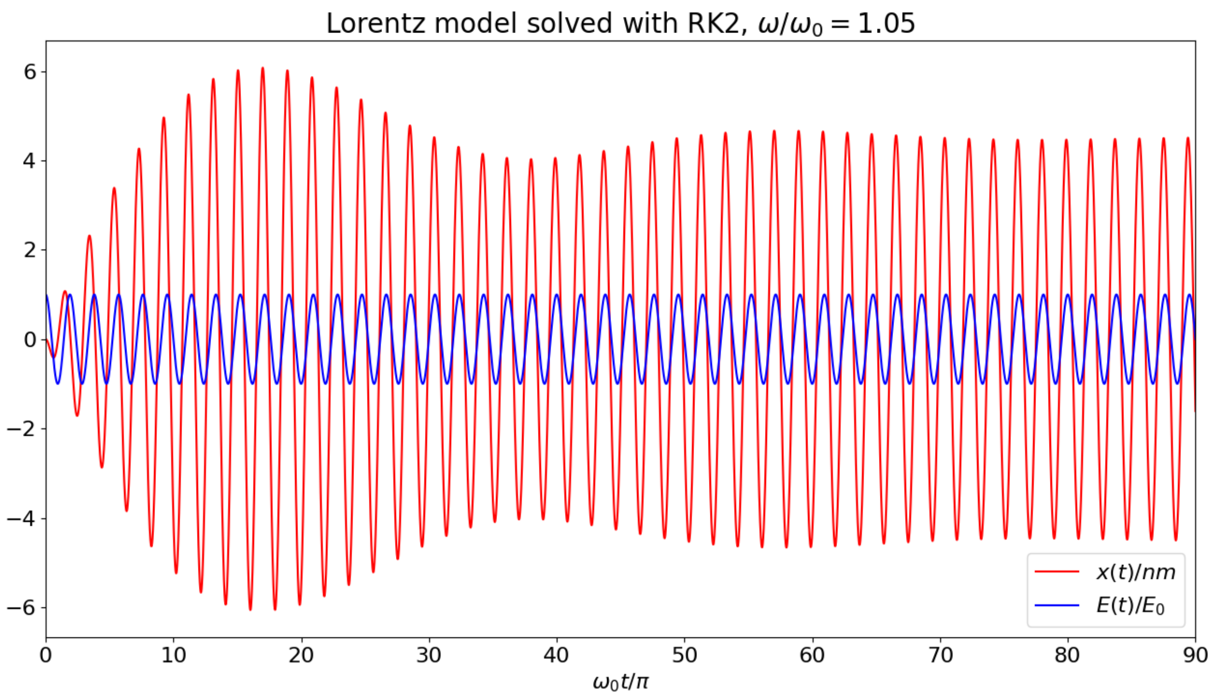
choose

$$\omega = 1.03\omega_0 \left(rad/s\right) \text{ and } E = E_0 \cos\left(\omega t\right) \ \& E_0 = 70\cdot 10^9 \left(V/m\right)$$



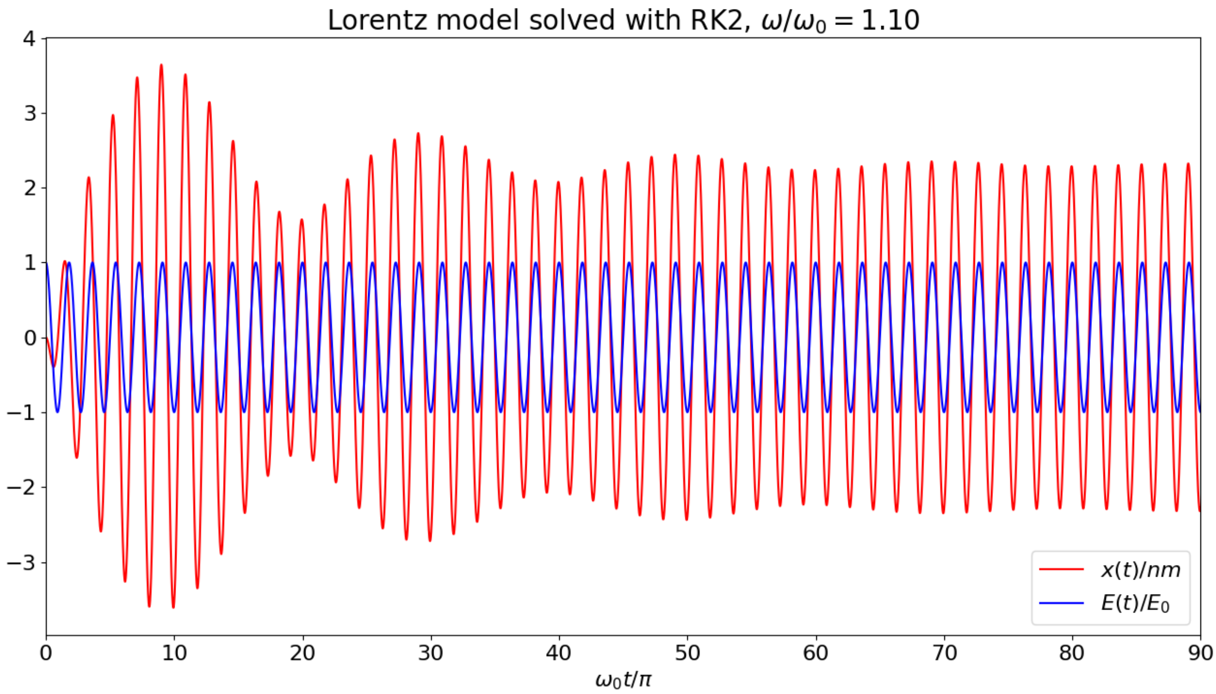
choose

$$\omega = 1.05\omega_0 \left(rad/s\right) \text{ and } E = E_0 \cos\left(\omega t\right) \ \& E_0 = 70\cdot 10^9 \left(V/m\right)$$



choose

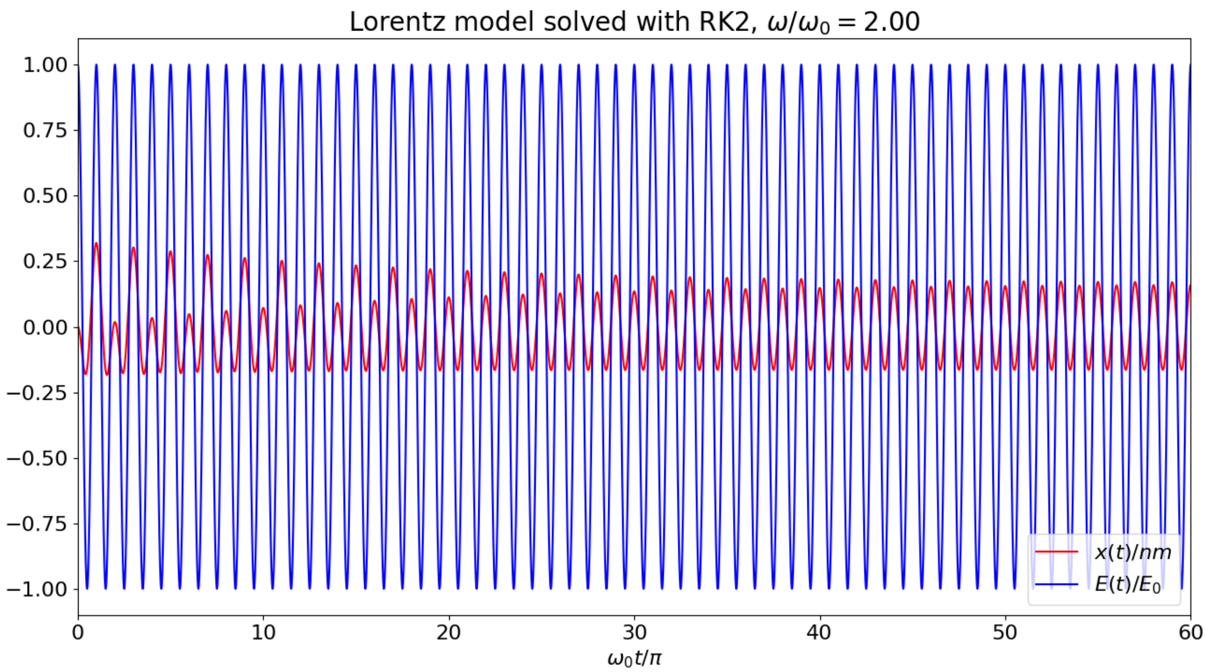
$\omega = 1.1\omega_0 \left(rad / s \right)$ and $E = E_0 \cos\left(\omega t \right)$ & $E_0 = 70 \cdot 10^9 \left(V / m \right)$



Case $(d)\, \omega \gg \omega_0$:

choose

$\omega = 2\omega_0 \left(rad / s \right)$ and $E = E_0 \cos\left(\omega t \right)$ & $E_0 = 70 \cdot 10^9 \left(V / m \right)$

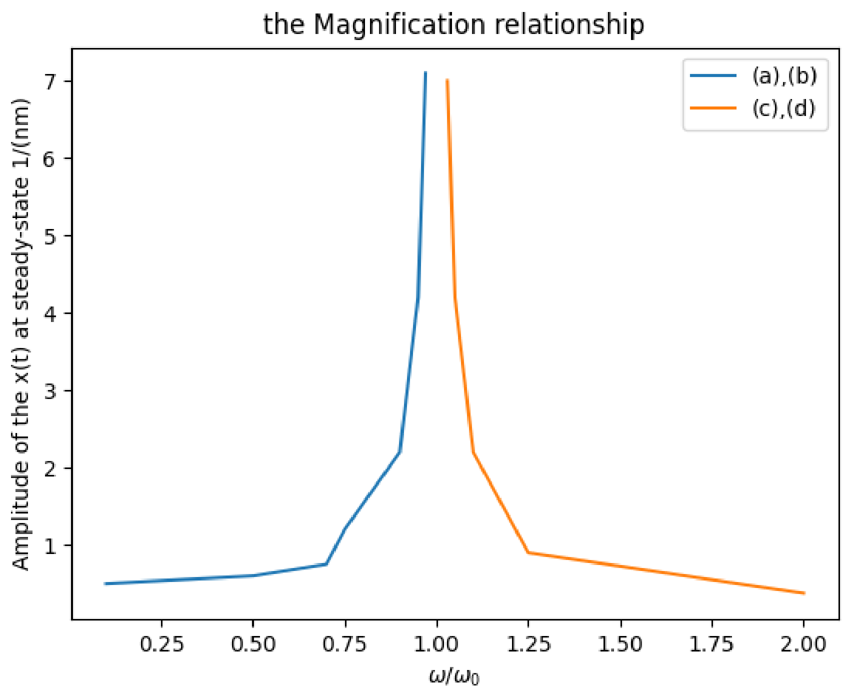


Conclusion of Problem 2

In $(a),(b)$ from problem 2, I observed that as the ω/ω_0 increase before 1, the amplitude of the solution increases too, and it will need more time to reach the steady state.

In $(c),(d)$ from problem 2, I observed that as the ω/ω_0 increase after 1, the amplitude of the solution decreases, and it will need less time to reach the steady state.

Visualize the magnification:



In $(a),(b)$ from problem 2, the relationship between steady-state response and the force applying by the time-dependent electric field is in phase. However, in $(c),(d)$ from problem 2 the relationship between them is out of phase.

Option advanced studies:

In reality, the laser beam in a spectroscopy is temporally pulsed.

for example:

$$E(t) = E_0 e^{-\left(\frac{t-t_0}{\Delta_t}\right)^2} \cos(\omega t) \tag{14}$$

Simulated the dynamical movement of an atom-bound electron in $NaCl$, and solve for the $x(t)$, as a function of time, under the light pulse with:

$$(i)\Delta_t^{-1} < \omega$$

$$(ii)\Delta_t^{-1} \sim \omega$$

$$(iii)\Delta_t^{-1} > \omega$$

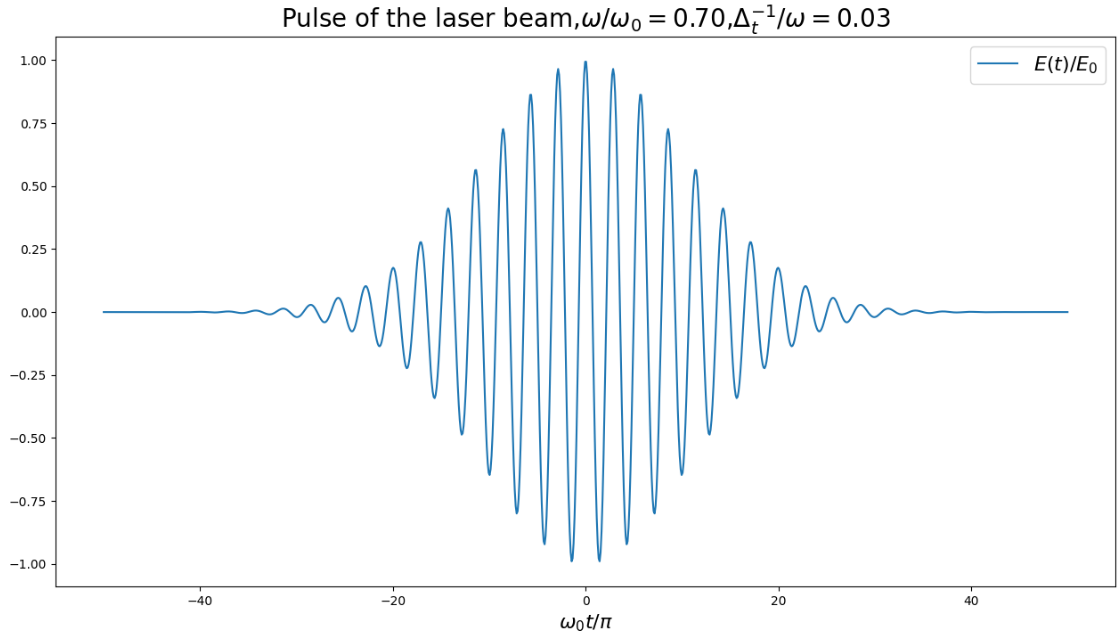
Solution:

In case $(i)\Delta_t^{-1} < \omega$, I choose $\frac{\Delta_t^{-1}}{\omega} = 0.03, \frac{\omega}{\omega_0} = 0.7$

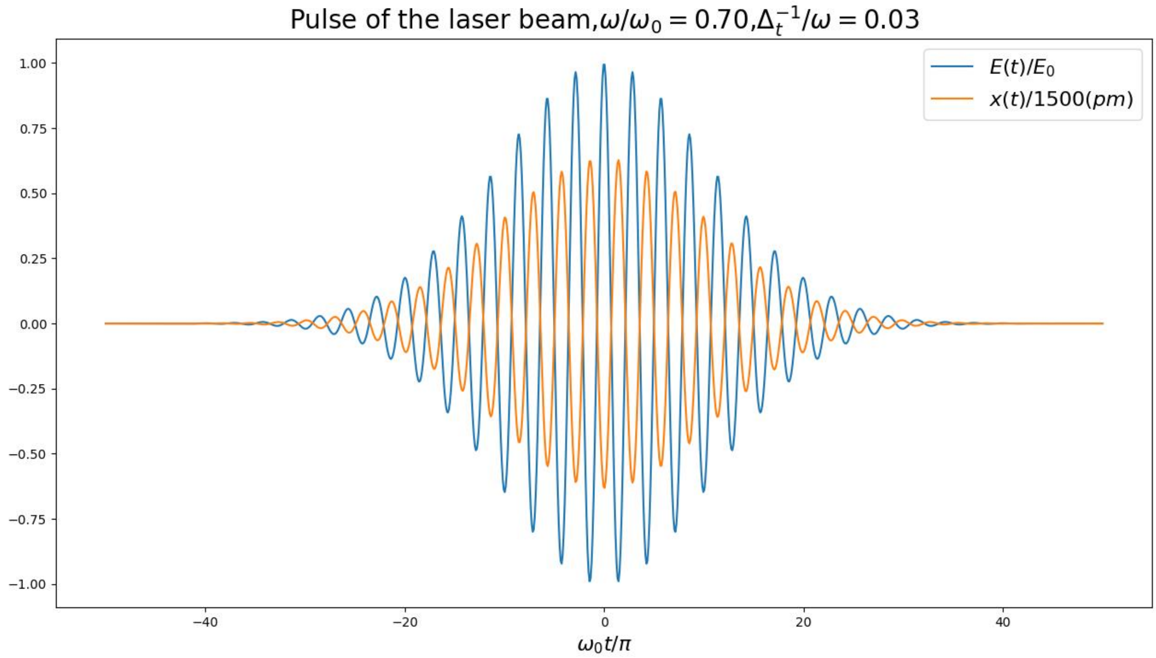
First, I try to construct the pulse in python code:

```
def Electric_field(ti):

    delta_t_inv=0.03*omega

    A_E=E_0*np.exp(-((ti)/(1/delta_t_inv))**2)

    return A_E*np.cos(omega*ti)

plt.plot(t,Electric_field(t*np.pi/omega_0)/E_0,label='$E(t)/E_0$')
```

And plot the pulse of the laser beam:

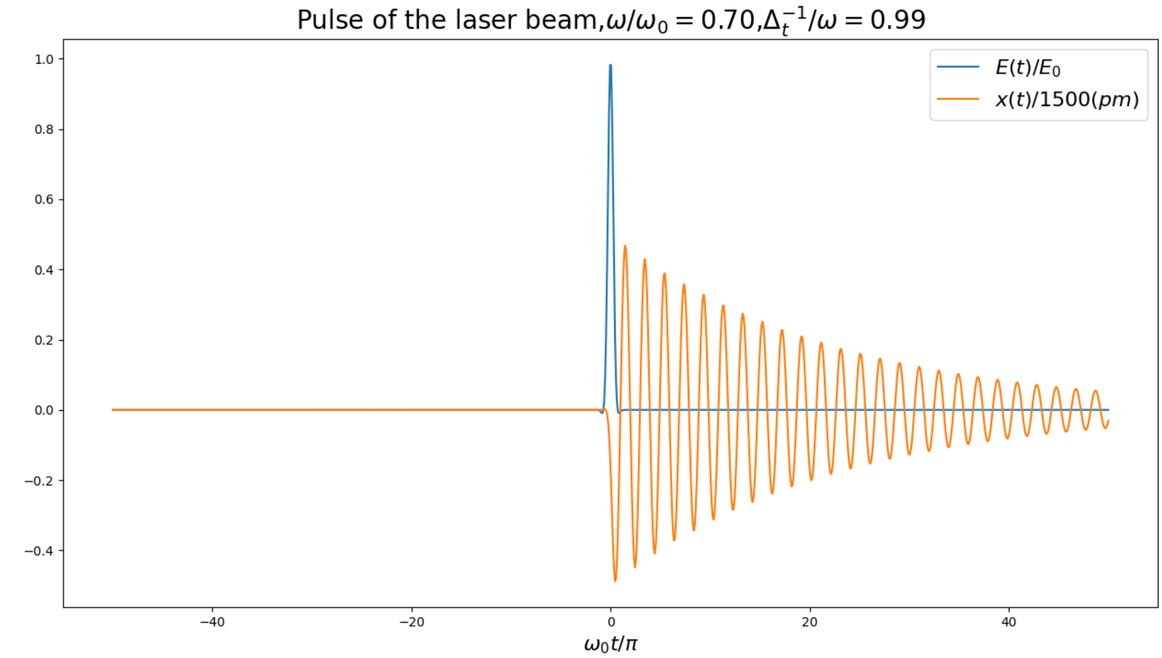


Second, I replace the electric field in Problem 2 with the pulse of the laser beam, and solve the ODE with Runge-Kutta method:

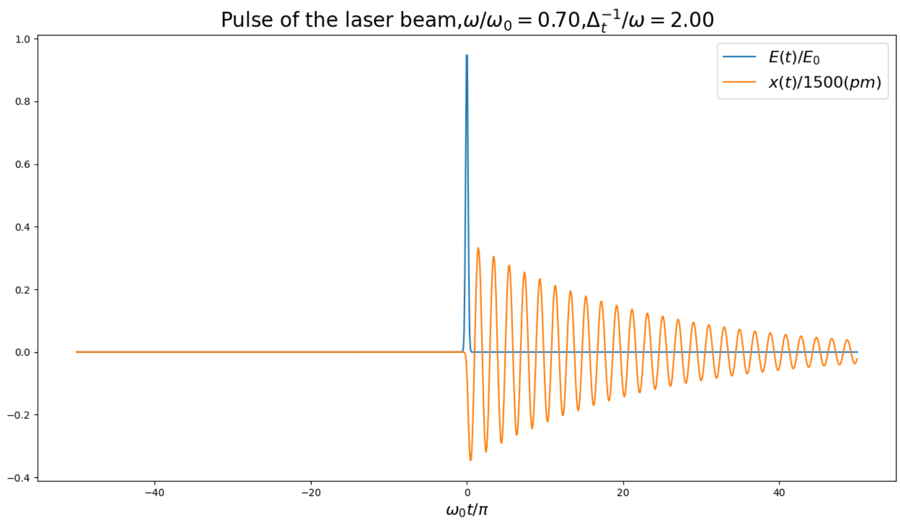


And we successfully solved the given question in case $(i)\Delta_t^{-1} < \omega$!

In case $(ii)\Delta_t^{-1} \sim \omega$, I choose $\frac{\Delta_t^{-1}}{\omega}=0.99, \frac{\omega}{\omega_0}=0.7$



In case $(iii)\Delta_t^{-1} > \omega$, I choose $\frac{\Delta_t^{-1}}{\omega}=2, \frac{\omega}{\omega_0}=0.7$



In both cases, the pulse of the laser beam seems to be a delta function, which simulates near at $t=0$. The solution of the ODE can be thought of as a boy is playing on the swing, and his parents just push him at the beginning.

Summary:

In problem 1, I learn how to fit the refractive index curve of the material and obtain the value of χ_{bg} 、γ, so that I can start the next step.

In problem 2, I used Runge-Kutta method to numerically solve the differential equation in Lorentz model with the time-dependent electric field.

In optional advanced study, I simulated the Lorentz model with the pulse of the laser beam, and successfully get the solution.

In this project, I learn how to use the ability of the computer to figure out the solution before the model reaches the steady-state, which is a little difficult for human to solve by basic calculation.

Feedback:

This course is absolutely the most impressive in this semester. I learn numerical differentiation、integration. Using FEM to solve PDE. Using Euler method and RK2 method to solve differential equation. Such skills are so interesting, and the algorithms are so astonishing. Many thanks to the professor's and teaching assistant's explanation!

Here is the code in this class: https://github.com/coherent17/physics_calculation

Additional practicing:

RLC circuit:

$$L\frac{d^2q}{dt^2}+R\frac{dq}{dt}+\frac{1}{C}q=0 \tag{14}$$

Divided by L on the both side:

$$\frac{d^2q}{dt^2}+\frac{R}{L}\frac{dq}{dt}+\frac{1}{LC}q=0 \tag{15}$$

Rewrite the as the coupled ODE:

$$\begin{cases}\dfrac{dq}{dt}=-i\\[2ex] \dfrac{d^2q}{dt^2}=-\dfrac{di}{dt}=-\dfrac{1}{LC}q-\dfrac{R}{L}\left(\dfrac{dq}{dt}\right)\end{cases}\Rightarrow\begin{cases}\dfrac{dq}{dt}=-i\\[2ex] \dfrac{di}{dt}=\dfrac{1}{LC}q-\dfrac{R}{L}i\end{cases} \tag{16}$$

We defined:

$$y_1=q, y_2=i \tag{17}$$

Substitute (17) into (16):

$$\begin{cases}\dfrac{dy_1}{dt}=-y_2\equiv g_1(y_2)\\[2ex] \dfrac{dy_2}{dt}=\dfrac{1}{LC}y_1-\dfrac{R}{L}y_2\equiv g_2(y_1,y_2)\end{cases} \tag{18}$$

By Runge-Kutta to solve y_1 and y_2:

$$\begin{cases}y_{1,i+1}\approx y_{1,i}+h\left(\dfrac{k_1}{2}+\dfrac{k_2}{2}\right)\\[2ex] k_1\equiv g_1(y_{2,i})\\[1ex] k_2\equiv g_1(y_{2,i}+hq_1)\end{cases}\begin{cases}y_{2,i+1}\approx y_{2,i}+h\left(\dfrac{q_1}{2}+\dfrac{q_2}{2}\right)\\[2ex] q_1\equiv g_2(y_{1,i},y_{2,i})\\[1ex] q_2\equiv g_2(y_{1,i}+hk_1,y_{2,i}+hq_1)\end{cases} \tag{19}$$

Code in python:

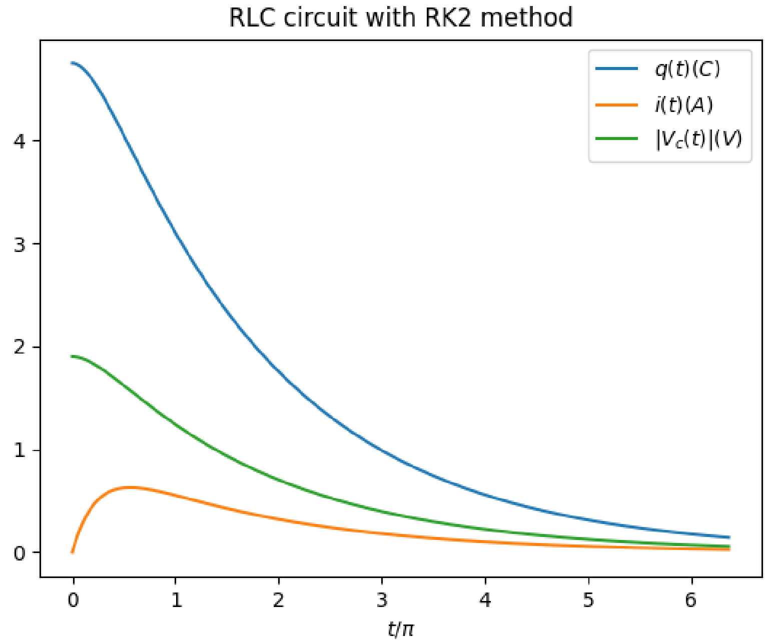
```
import numpy as np
import matplotlib.pyplot as plt

#parameter:
e=1.9 #charge voltage (volt)
R=2.5 #(ohm)
L=1.7 #(h)
C=2.5 #(F)
N=2000
h=0.01
t=np.arange(N)*h

#initial condition:
q0=C*e
i0=0.0

def g1(y1,y2):
    return (-y2)

def g2(y1,y2):
    return 1/(L*C)*y1-(R/L)*y2

#calculate the value of the next moment by RK2 m
ethod
def y_rk2(y1,y2):#with (w1,w2,alpha,beta) = (0.5
,0.5,1,1)
    k1=g1(y1,y2)
    q1=g2(y1,y2)
    k2=g1(y1+h*k1,y2+h*q1)
    q2=g2(y1+h*k1,y2+h*q1)
    y1_prime=y1+h*(0.5*k1+0.5*k2)
    y2_prime=y2+h*(0.5*q1+0.5*q2)
```

```python
    return y1_prime,y2_prime

def SHO():
    q=[]
    i=[]
    V_c=[]
    q.append(q0)
    i.append(i0)
    V_c.append(q0/C)
    for j in range(0,N-1):
        a,b=y_rk2(q[j],i[j])
        q.append(a)
        i.append(b)
        V_c.append(np.abs(a/C))
    return q,i,V_c

def visualize(q,i,V_c):
    plt.plot(t/np.pi, q, label="$q(t) (C)$")
    plt.plot(t/np.pi, i, label="$i(t) (A)$")
    plt.plot(t/np.pi, V_c, label="$|V_c(t)| (V)$")
    plt.title("RLC circuit with RK2 method")
    plt.xlabel("$t/\pi$")
    plt.xticks(fontsize=10)
    plt.yticks(fontsize=10)
    plt.legend()
    plt.show()

q,i,V_c=SHO()
visualize(q,i,V_c)
```

Results:

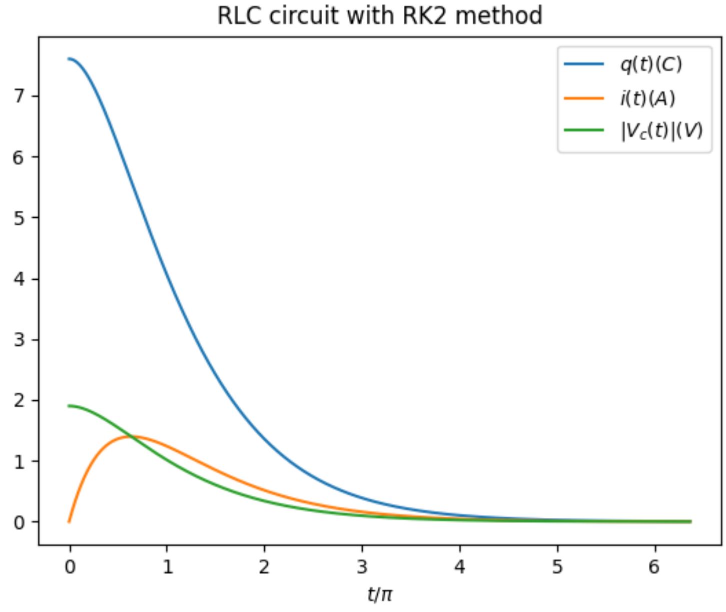
$< case\ 1 >$ $overdamping$

$$L = 1.7(H), C = 2.5(F), R = 2.5(\Omega), \varepsilon = 1.9(V)$$



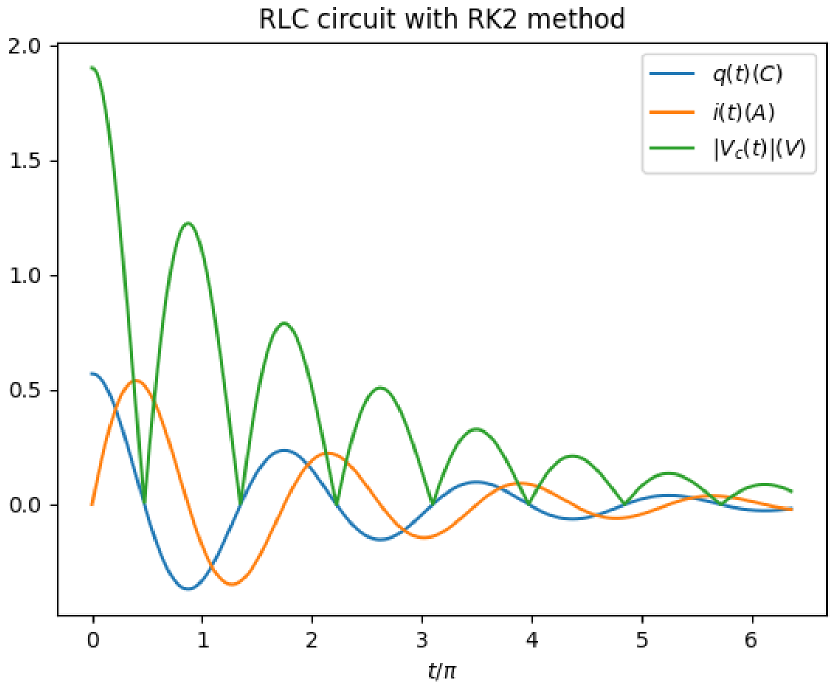
$< case\ 2 >$ $criticaldamping$

$$L = 1(H), C = 4(F), R = 1(\Omega), \varepsilon = 1.9(V)$$



$<case\ 3>\ \ underdamping$

$L = 2.5(H), C = 0.3(F), R = 0.8(\Omega), \varepsilon = 6.33(V)$



And now we apply AC supplier to RLC circuit, solve the ODE again!

By KVL, we have:

$$L\frac{d^2q}{dt^2} + R\frac{dq}{dt} + \frac{1}{C}q = \varepsilon_0 \cos(\omega t) \tag{20}$$

Divided L on the both side:

$$\frac{d^2q}{dt^2} + \frac{R}{L}\frac{dq}{dt} + \frac{1}{LC}q = \frac{\varepsilon_0}{L}\cos(\omega t) \tag{21}$$

Rewrite as the coupled ODE:

$$\begin{cases} \dfrac{dq}{dt} = -i \\ \dfrac{di}{dt} = \dfrac{1}{LC}q - \dfrac{R}{L}i - \dfrac{\varepsilon_0}{L}\cos(\omega t) \end{cases} \tag{22}$$

We defined:

$$y_1 = q, y_2 = i \tag{23}$$

Substitute (23) into (22):

$$\begin{cases} \dfrac{dy_1}{dt} = -y_2 \equiv g_1(y_2) \\ \dfrac{dy_2}{dt} = \dfrac{1}{LC} y_1 - \dfrac{R}{L} y_2 - \dfrac{\varepsilon_0}{L} \cos(\omega t) \equiv g_2(y_1, y_2) \end{cases} \tag{24}$$

By Runge-Kutta to solve y_1 and y_2:

$$\begin{cases} y_{1,i+1} \approx y_{1,i} + h\left(\dfrac{k_1}{2} + \dfrac{k_2}{2}\right) \\ k_1 \equiv g_1(y_{2,i}) \\ k_2 \equiv g_1(y_{2,i} + hq_1) \end{cases} \begin{cases} y_{2,i+1} \approx y_{2,i} + h\left(\dfrac{q_1}{2} + \dfrac{q_2}{2}\right) \\ q_1 \equiv g_2(y_{1,i}, y_{2,i}) \\ q_2 \equiv g_2(y_{1,i} + hk_1, y_{2,i} + hq_1) \end{cases} \tag{25}$$

Code in python:

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

#parameter:
e=100 #charge voltage (volt)
R=2.5 #(ohm)
L=1.7 #(h)
C=2.5 #(F)
N=2000
h=0.01
t=np.arange(N)*h
omega=5

#initial condition:
```

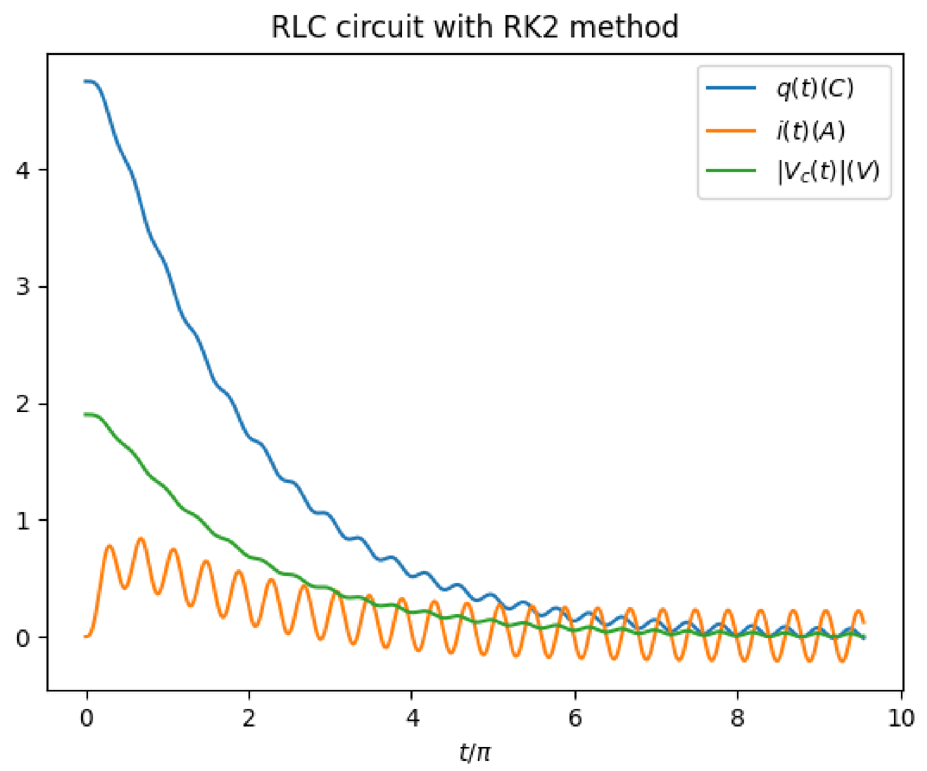
```python
q0=C*e
i0=0.0

def g1(y1,y2):
    return (-y2)

def g2(y1,y2,ti):
    return 1/(L*C)*y1-(R/L)*y2-e/L*np.cos(omega*ti)


#calculate the value of the next moment by RK2 method
def y_rk2(y1,y2,ti):#with (w1,w2,alpha,beta) = (0.5,0.5,1,1)
    k1=g1(y1,y2)
    q1=g2(y1,y2,ti)
    k2=g1(y1+h*k1,y2+h*q1)
    q2=g2(y1+h*k1,y2+h*q1,ti)
    y1_prime=y1+h*(0.5*k1+0.5*k2)
    y2_prime=y2+h*(0.5*q1+0.5*q2)
    return y1_prime,y2_prime

def SHO():
    q=[]
    i=[]
    V_c=[]
    q.append(q0)
    i.append(i0)
    V_c.append(q0/C)
    for j in range(0,N-1):
        a,b=y_rk2(q[j],i[j],t[j])
        q.append(a)
        i.append(b)
        V_c.append(np.abs(a/C))
    return q,i,V_c
```

```python
def visualize(q,i,V_c):
    plt.plot(t/np.pi, q, label="$q(t) (C)$")
    plt.plot(t/np.pi, i, label="$i(t) (A)$")
    plt.plot(t/np.pi, V_c, label="$|V_c(t)| (V)$")
    plt.title("RLC circuit with RK2 method")
    plt.xlabel("$t/\pi$")
    plt.xticks(fontsize=10)
    plt.yticks(fontsize=10)
    plt.legend()
    plt.show()
q,i,V_c=SHO()
visualize(q,i,V_c)
```

Result:

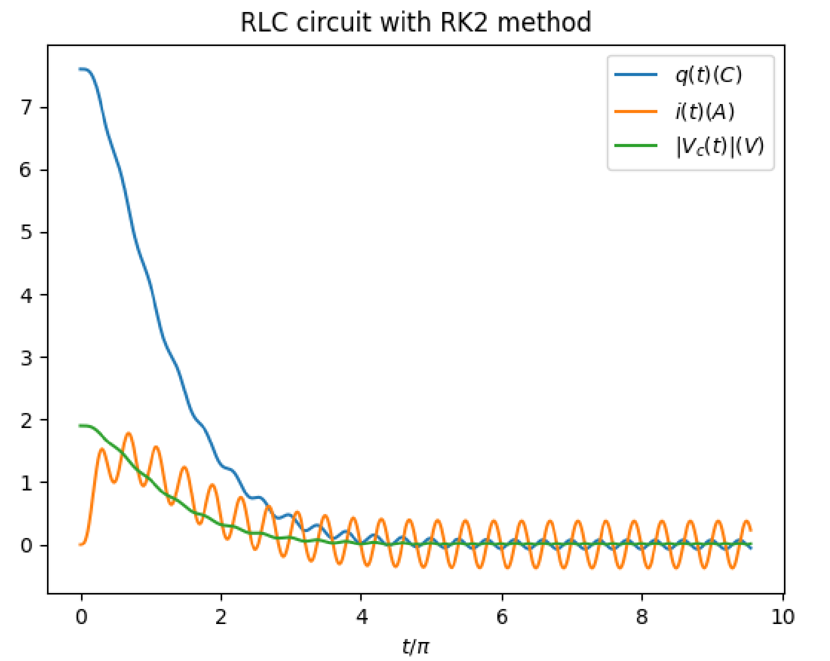
$< case\ 1 >\ \ overdamping$

$$L = 1.7(H), C = 2.5(F), R = 2.5(\Omega), \varepsilon = 1.9(V), \omega = 5(1/s)$$



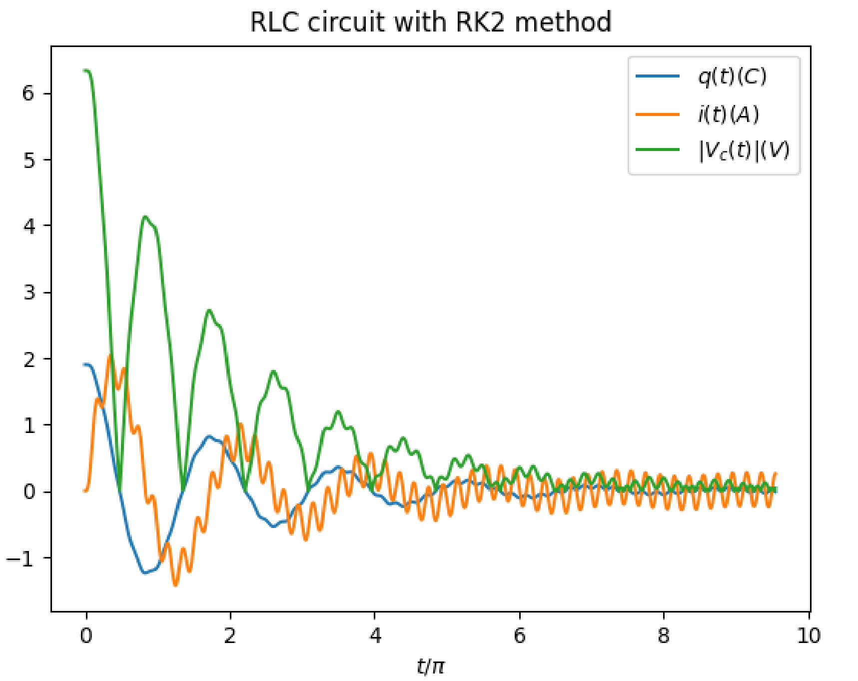
$< case\ 2 >\ \ critical damping$

$$L=1(H), C=4(F), R=1(\Omega), \varepsilon=1.9(V), \omega=5(1/s)$$

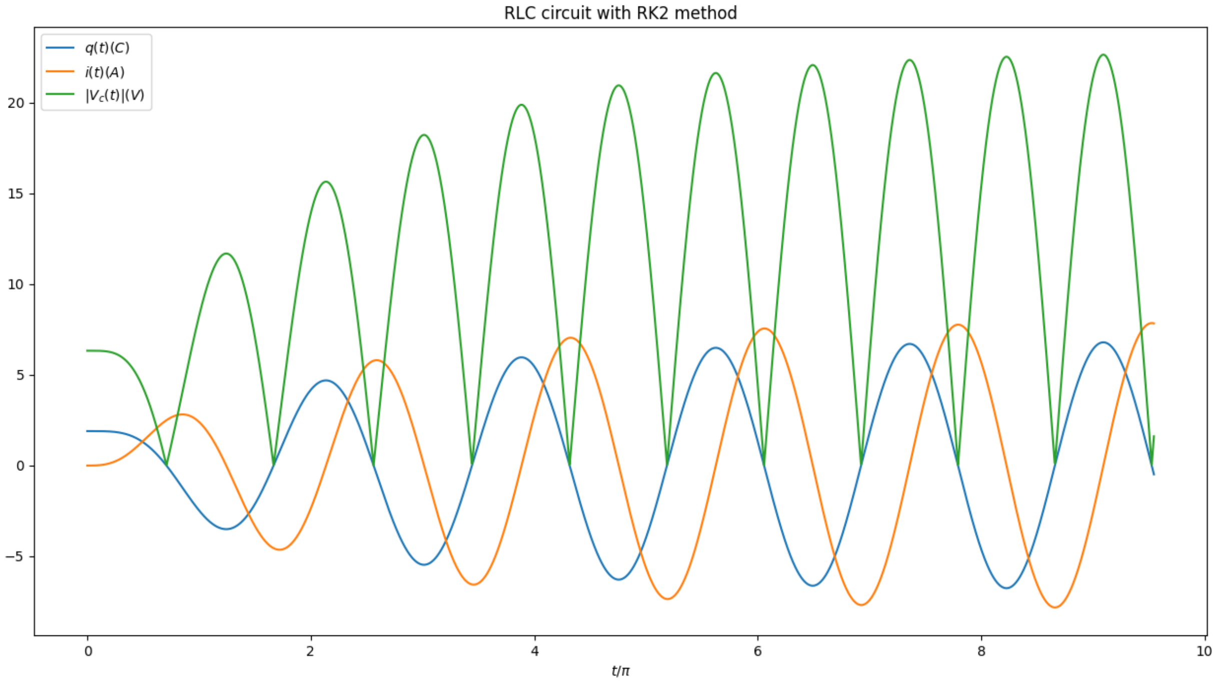


$< case\ 3 >\ \ underdamping$

$$L=2.5(H), C=0.3(F), R=0.8(\Omega), \varepsilon=6.33(V), \omega=10(1/s)$$



What happens if the frequency of the AC supplier is $\sqrt{\frac{1}{LC}}$?



The resonance happens.

Explanation the procedure from transient state to steady state.

At first, the capacitor charge and start to discharge, and the AC supplier will charge the capacitor. As we can see in the case 3: underdamping, the amplitude keeps decreasing, until some period, and the amplitude reaches a constant. This is my explanation: In one period, the charge loss in capacitor is more than the AC supplier supply. Therefore, in one period, the net charge store in capacitor is decreased. Will it decrease to zero? It might decrease until the input charges from AC supplier are equal to the output charge from discharging, and that's why there exists a steady oscillation at final, which is the steady-state. This damping system is very similar to our final project: Lorentz model. And that's really interesting to compare between them.