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DYNAMICS OF A DAMPED CLASSICAL HARMONIC OSCILLATOR: GUIDE TO BEGINNER

Chemistry

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ABSTRACT

In this review article I have reproduced the dynamics of a damped classical harmonic oscillator (DCHO) in the under damped regime by solving the second order differential equation (SODE) for the oscillator analytically and numerically using the popular RK4 method. The combined plot of position and energy vs. time for the DCHO reveals that the energy dissipates rapidly as the oscillator passes through the equilibrium position compared to the extreme position.

KEYWORDS

DCHO, SODE, RK4, FORTRAN

INTRODUCTION

Oscillator is one of the most extensively studied systems in physics and physical chemistry. Examples include from suspension of vehicles in the classical world to covalent bond in the quantum world[1]. Over centuries scientists have widely studied systems involving classical harmonic oscillator (CHO) incorporating damping and or driving force. CHO associated with both damping and fluctuating driving force is an excellent tool for theoretical chemists working in the field of barrier crossing process using in silico experiments[2,3,4]. Remarkable work has been done and is being done in this field. Young researchers may proceed with this topic as huge scope is there. I hope this article will be able to guide the beginners.

Classical Harmonic Oscillator (CHO)

The equation of motion for a CHO is guided by the Hooke's law & Newton's 2nd law of motion

$$F_r = -\nabla V = -kx$$

$$\text{or, } ma = m\ddot{x} = m\frac{d^2x}{dt^2} = -kx$$

$$\text{or, } \ddot{x} + \frac{k}{m}x = 0 \quad \dots (1)$$

where F_r is the force experienced by the oscillator which tries to restore the oscillator to its equilibrium position, k is the spring constant, $V(x) = \frac{1}{2}kx^2$ is the potential energy of the one dimensional(1D) oscillator, m is the mass of the oscillator and $x = x(t)$ is the position of the oscillator at time t and $x = 0$ is the stable equilibrium position.

Now, we will solve the quadratic equation (1) using standard technique. Euler developed the method of solving this type of equation. Let, $x(t) = C \times e^{\lambda t}$ be the trial solution. Executing the 1st and 2nd order derivation of the trial solution we get

$v(t) = \dot{x}(t) = \lambda Ce^{\lambda t}$ and $a(t) = \ddot{x}(t) = \lambda^2 Ce^{\lambda t}$

and then putting the above expressions in equation (1) we have,

$$\lambda^2 Ce^{\lambda t} + \frac{k}{m}Ce^{\lambda t} = 0 \quad \text{or, } \left(\lambda^2 + \frac{k}{m}\right)Ce^{\lambda t} = 0$$

$$\because Ce^{\lambda t} \neq 0 \;\; \therefore \lambda^2 + \frac{k}{m} = 0 \;\; \text{or, } \lambda_{1,2} = \pm i\sqrt{\frac{k}{m}}$$

$$\therefore x(t) = C_1 e^{+i\sqrt{\frac{k}{m}}t} + C_2 e^{-i\sqrt{\frac{k}{m}}t}$$

Using, $e^{\pm i\theta} = \cos(\theta) \pm i \times \sin(\theta)$, we have

$$x(t) = C_1\left\{\cos\left(\sqrt{\frac{k}{m}}t\right) + i \times \sin\left(\sqrt{\frac{k}{m}}t\right)\right\} + C_2\left\{\cos\left(\sqrt{\frac{k}{m}}t\right) - i \times \sin\left(\sqrt{\frac{k}{m}}t\right)\right\}$$

$$= (C_1 + C_2)\cos\left(\sqrt{\frac{k}{m}}t\right) + i(C_1 - C_2)\sin\left(\sqrt{\frac{k}{m}}t\right)$$

$$= P\cos\left(\sqrt{\frac{k}{m}}t\right) + Q\sin\left(\sqrt{\frac{k}{m}}t\right)$$

Considering $P = A\sin(\varphi)$ and $Q = A\cos(\varphi)$, we have

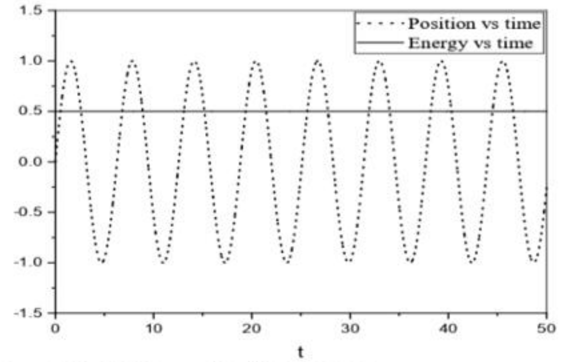
$$x(t) = A\sin(\varphi)\cos(\omega t) + A\cos(\varphi)\sin(\omega t) = A\sin(\omega t + \varphi) \quad \dots (2)$$

where A is the amplitude, $\omega = 2\pi\nu = \sqrt{\frac{k}{m}}$ is the angular frequency and $\nu = \frac{1}{T} = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$ is the natural frequency of the oscillator and T the time period is the time required for one complete oscillation. The energy of the 1D CHO can be determined easily using equation 2,

$$E = E_K + E_P = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2A^2 \quad \dots (3)$$

The position varies periodically as evident from equation 2 and the energy expression in equation 3 reveals that the energy of a simple harmonic oscillator which is neither driven nor damped remains constant. Solving the CHO numerically using RK4 method[5,6] in FORTRAN program we get the same result (Figure 1).

Figure 1:



Damped Classical Harmonic Oscillator (DCHO)

The inertial force ($F = m\ddot{x}$) is opposed by the restoring ($F_r = -kx$) and the frictional ($F_f = -\mu\dot{x}$) forces,

$$m\ddot{x} = -kx - \mu\dot{x} \;\; \text{or, } \ddot{x} + \frac{\mu}{m}\dot{x} + \frac{k}{m}x = 0 \quad \dots (4)$$

The equation is linear, homogeneous; second order differential equation (SODE) with constant coefficients. We will now solve equation 4 in the way as done in the previous section.

Let, $x(t) = C \times e^{\lambda t}$ be the trial solution. Executing the 1st and 2nd order derivation of the trial solution we get

$v(t) = \dot{x}(t) = \lambda Ce^{\lambda t}$ and $a(t) = \ddot{x}(t) = \lambda^2 Ce^{\lambda t}$.

Putting in equation 4 we have,

$$\lambda^2 Ce^{\lambda t} + \frac{\mu}{m}\lambda Ce^{\lambda t} + \frac{k}{m}Ce^{\lambda t} = 0$$

$$\text{or, } \left(\lambda^2 + \frac{\mu}{m}\lambda + \frac{k}{m}\right)Ce^{\lambda t} = 0$$

$\because Ce^{\lambda t} \neq 0 \quad \therefore \lambda^2 + \frac{\mu}{m}\lambda + \frac{k}{m} = 0$ ... This is called the characteristic equation.

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It is a quadratic equation in normal form. Solving we have, $\lambda_{1,2} = -\frac{\mu}{2m} \pm \sqrt{(\frac{\mu}{2m})^2 - \frac{k}{m}}$

Let, $\xi = \frac{\mu}{2m}$ and we know, $\omega = \sqrt{\frac{k}{m}}$,

$$\therefore \lambda_{1,2} = -\xi \pm \sqrt{\xi^2 - \omega^2} \quad ...(5)$$

Depending on the values of ξ and ω, three cases may arise. We will proceed with only one among the three, $\xi < \omega$, which represents the under damped regime. In this case the discriminant of equation 5 is negative and the roots of the equation $\lambda_{1,2}$ will be complex.

$$\therefore x(t) = C_1 e^{\left(-\xi + \sqrt{\xi^2-\omega^2}\right)t} + C_2 e^{\left(-\xi - \sqrt{\xi^2-\omega^2}\right)t}$$
$$= e^{-\xi t}\{C_1 e^{\left(+\sqrt{\xi^2-\omega^2}\right)t} + C_2 e^{\left(-\sqrt{\xi^2-\omega^2}\right)t}\}$$
$$= e^{-\xi t}\{C_1 e^{+i\nu t} + C_2 e^{-i\nu t}\}$$

where, $\nu = \sqrt{\omega^2 - \xi^2}$ is the natural frequency of the damped oscillator.

Let, $C_1 = a_1 e^{+i\varphi_1}$ and $C_2 = a_2 e^{+i\varphi_2}$

$$\therefore x(t) = e^{-\xi t}\{a_1 e^{+i\varphi_1} e^{+i\nu t} + a_2 e^{+i\varphi_2} e^{-i\nu t}\}$$
$$= e^{-\xi t}\{a_1 e^{+i(\varphi_1+\nu t)} + a_2 e^{+i(\varphi_2-\nu t)}\}$$
$$= e^{-\xi t}[\{a_1\cos(\varphi_1+\nu t) + i a_1 sin(\varphi_1+\nu t)\} + \{a_2\cos(\varphi_2-\nu t) + i a_2 sin(\varphi_2-\nu t)\}]$$
$$= e^{-\xi t}\{a_1\cos(\varphi_1+\nu t) + a_2\cos(\varphi_2-\nu t)\} + i e^{-\xi t}\{a_1 sin(\varphi_1+\nu t) + a_2 sin(\varphi_2-\nu t)\} \quad ...(6)$$

The above expression is the solution of the under damped classical harmonic oscillator. The first part of the solution is real while the second one is imaginary. The imaginary part must disappear, which implies

$$a_1 sin(\varphi_1+\nu t) + a_2 sin(\varphi_2-\nu t) = 0$$

or, $a_1 sin(\varphi_1+\nu t) = -a_2 sin(\varphi_2-\nu t)$

$$= a_2 sin(-\varphi_2+\nu t)$$
$$\therefore a_1 = a_2 \text{ and } \varphi_1 = -\varphi_2$$

Thus we can rewrite equation 6 as

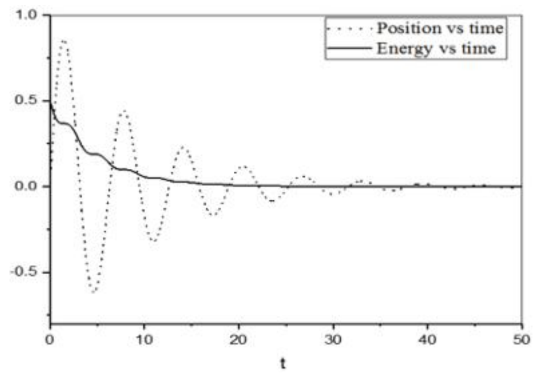
$x(t) = e^{-\xi t}\{a_1\cos(\varphi_1+\nu t) + a_1\cos(-\varphi_1-\nu t)\}$

$= e^{-\xi t}\{a_1\cos(\varphi_1+\nu t) + a_1\cos(\varphi_1+\nu t)\}$

or, $x(t) = 2a_1 e^{-\xi t}\cos(\varphi_1+\nu t) \quad ...(7)$

Equation 7 is the final solution of the DCHO in the under damped regime and the expression predicts Figure 2. The cosine term maintains the periodicity and the exponential term carries the signature of the damping. Energy is drained from the oscillator in every oscillation and ultimately it comes to rest.

Figure 2:



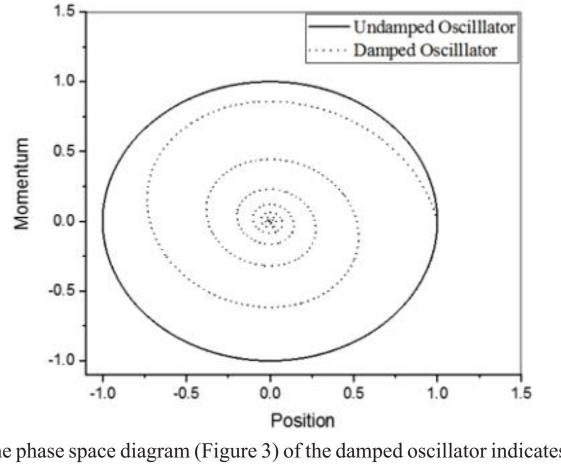
Solving the DCHO numerically using RK4 method[5,6] in FORTRAN program we get the same result (Figure 2). I am supplying the core part of the FORTRAN code which may help an interested apprentice.

```
ak1=fp(q)*h
al1=fq(p)*h
ak2=fp(q+al1/2)*h
al2=fq(p+ak1/2)*h
ak3=fp(q+al2/2)*h
al3=fq(p+ak2/2)*h
ak4=fp(q+al3)*h
al4=fq(p+ak3)*h
q=q0+(al1+al2*2+al3*2+al4)/6
p=p0+(ak1+ak2*2+ak3*2+ak4)/6
t=t+h
q0=q
p0=p
```

where, the functions are defined as fp(q)= -k*q-μ*p and fq(p)= p/m, t is the time, q is the coordinate and p is the momentum.

The combined plot of position and energy vs. time for the DCHO reveals that the energy dissipates rapidly as the oscillator passes through the equilibrium position compared to the extreme position and the amplitude of the oscillator falls exponentially (Equation 7) to zero after a certain amount of time.

Figure 3:



The phase space diagram (Figure 3) of the damped oscillator indicates that the oscillator comes to equilibrium after a certain amount of time as it losses energy heterogeneously due to damping and ultimately both the coordinate and momentum domain quenches.

CONCLUSION

The energy of the oscillator dissipates rapidly as it passes through the equilibrium position compared to the extreme position. The result is obvious since the oscillator is slow near the turning points where the kinetic energy is minimum and fast as it crosses the equilibrium position where the kinetic energy is maximum thereby experiences more friction. The amplitude of the DCHO however experiences an exponential decay with time.

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Conflicts of Interest: None

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