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Research Article

GREEN'S FUNCTION SOLUTION FOR THE ITINERANT OSCILLATOR MODEL FOR FLUIDS

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ABSTRACT

The basic equations for the itinerant oscillator model for fluids proposed by Sears and modified by Nakahara and Takahashi (1966), and Damle *et al.,* (1968) are solved using the method of Green's functions solutions. Supposing the forces of interaction operating among the molecules to be either exponential or oscillatory, we have found the solutions of the equations proposed by Sears (1965).

The two solutions for the value of $R_0(t)$, the position of the moving molecule, differ in the sense that in one case when the force is exponential the value of $R_0(t)$ depends on well known parameters, whereas when the force is oscillatory, the value of modified $R_0(t)$ contains some imaginary terms. Under the condition $t = t_0$, the two solutions are practically identical.

INTRODUCTION

Sears (1965) had proposed the itinerant oscillator model of liquids in which he introduced the concept of centre of oscillation defined in such a way that the motion of an atom relative to its centre represents its thermal oscillation, whereas the motion of the centre of oscillation represents the diffuse motion of the atom. The centre of oscillation was defined as the average position of the central atom. The equation of motion of the central atom was written in terms of ω_0 which is the frequency of oscillation of the central atom, μ as a friction constant, and $\mathrm{A}(t)$ as the random force whose average may be zero.

It was later pointed out (Nakahara *et al.*, 1966) that Sear's treatment was inconsistent with the well accepted second fluctuation-dissipation theorem. Damle *et al.,* (1968) pointed out the error in the treatment of Nakahara and Takahashi (1966), and also brought out a striking feature of Sear's model: it does not obey the third law of Newton; it violates the equality of action and reaction. The Sear's model and other models were re-examined (Cardi *et al.*, 1971) and various ways were proposed to overcome the deficiencies.

However, before we develop our ideas on such a model, it will be appropriate to understand (Hill 1963, Wyllie 1971) that with each molecule in a substance is associated a least polyhedron whose faces are the normal bisectors of the lines joining the centre of that molecule to the centers of a number of neighboring molecules. These neighbors at any moment form a cage, and the motion of each molecule is dominated by its interaction with the members of its cage. In a solid the membership of a cage is constant for periods very long compared with the principle periods of oscillation of the translation and rotation of each molecule. In a liquid, the following points are to be carefully noted.

- The membership of the neighboring cages is frequently exchanged.

- Each cage has titubant diffusive motion corresponding to the fluidity of the surrounding medium.

This way of looking at the structure and motion of a liquid gives rise to what is known as the itinerant oscillator model of molecular motion in which each molecule is assumed to make a damped oscillation about an equilibrium position which itself executes a diffuse motion. The model may be applied to angular (Hill, 1963) as well as to linear (Sears, 1965, 1967) motion of the molecule.

Itinerant oscillator model has also been used to study the contribution of particle inertial effects to resonance in ferrofluids (Fannin and Coffey, 1995). Similarly non-Fermi liquid nature of the normal state of itinerant-electron ferromagnets has been studied (Pfleiderer *et al.*, 2001).

A review article (Coffey *et al.*, 2003) on itinerant oscillator models of fluids gives extensive details on how the model can be applied to different types of fluids. Many details are given as to how to study different types of problems, and a large number of references are given for further reading and understanding of the subject matter. In most of the cases small oscillation harmonic potential approximation is used, and in some cases attempts were made to generalize the model to include anharmonic potential. Another application of the model is the relaxation of ferrofluids (Shliomis, 1974).

Now the forces $A(t)$ and $B(t)$ used by Sears (1965, 1967) are stationary stochastic forces. Similarly different types of forces have been used by others (Coffey *et al*., 2003) also in studying different problems. In some cases the forces $\mathrm{A}(t)$ and $\mathrm{B}(t)$ are random forces whose average could be zero.

In the calculations presented in this manuscript, we have used simple oscillating forces in one set of calculations, and forces exponentially decreasing in the other set of calculations. This is based on the assumption that in a system enclosed in a box a molecule interacts with all the other molecules and the forces of interaction should be either oscillating with time or decreasing with time. Green's function solutions have been used to study and solve the equations of motion.

THEORY

The equations of motion used by Sears as per the model proposed by him are,

$$\ddot{R}_0(t)+\mu\dot{R}_0(t)+\omega_0^2\{R_0(t)-R(t)\}=\mathrm{A}(t) \quad \text{......} (1)$$

$$\ddot{R}(t)+\upsilon\dot{R}(t)=\mathrm{B}(t) \quad \text{......} (2)$$

Where R_0 is the position of the moving molecule and R that of its temporary centre of oscillation, and μ and υ are friction constants, ω_0 is the frequency of oscillation. In general $\mu\neq\upsilon$. The forces $\mathrm{A}(t)$ and $\mathrm{B}(t)$ used by Sears are stationary stochastic forces. But here we will use simple oscillating forces in one set of calculations, and forces exponentially decreasing with time in the other set of calculations. This is based on the assumption that in a system enclosed in a box a molecule interacts with all the other molecules and the forces of interaction should be either oscillating with time or decreasing with time.

Now equations (1) and (2) can be solved by giving suitable values to $\mathrm{A}(t)$ and $\mathrm{B}(t)$. First we consider forces that decrease exponentially with time such that we can write,

$$\mathrm{A}(t)=\mathrm{A}_0e^{-\gamma t}$$
$$\mathrm{B}(t)=\mathrm{B}_0e^{-\beta t} \quad \text{......} (3)$$

Equations (1) and (2) can be written in the form,

$$\ddot{R}_0(t)+\mu\dot{R}_0(t)+\omega_0^2R_0(t)=\mathrm{A}_0e^{-\gamma t}+\omega_0^2R(t)=f(t) \quad \text{......} (4)$$

$$\ddot{R}(t)+\upsilon\dot{R}(t)=\mathrm{B}_0e^{-\beta t} \quad \text{......} (5)$$

The mathematical solution of Equation (4) in terms of Green's functions is given by (Byron and Fuller, 1970),

$$R_0(t) = PR_{01}(t) + QR_{02}(t) + \int_{-\infty}^{+\infty} G(t,t')f(t')dt' \quad \text{.......} \quad (6)$$

Where P and Q are to be chosen to satisfy the boundary conditions, and

$$R_{01}(t) = e^{-\frac{\mu t}{2}} \sin\left[\left(\omega_0^2 - \frac{\mu^2}{4}\right)^{\frac{1}{2}} t\right] \quad \text{.......} \quad (7)$$

$$R_{02}(t) = e^{-\frac{\mu t}{2}} \cos\left[\left(\omega_0^2 - \frac{\mu^2}{4}\right) t\right]$$

$$f(t) = \mathrm{A}_0 e^{-\gamma t} + \omega_0^2 R(t)$$

Green's function $G(t,t')$ can be expressed by the integral,

$$G(t,t') = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{e^{-ik(t-t')}}{(k-k_1)(k-k_2)}dk \quad \text{.......} \quad (8)$$

Where

$$k_1 = \left(\omega_0^2 - \frac{\mu^2}{4}\right)^{\frac{1}{2}} - i\frac{\mu}{2} = \alpha - i\frac{\mu}{2}$$

$$k_2 = -\left(\omega_0^2 - \frac{\mu^2}{4}\right)^{\frac{1}{2}} - i\frac{\mu}{2} = -\alpha - i\frac{\mu}{2}$$

$$\omega_0 > \frac{\mu}{2} \quad \text{and} \quad \left(\omega_0^2 - \frac{\mu^2}{4}\right)^{\frac{1}{2}} = \alpha$$

Now for $t > t'$, we can evaluate the integral,

$$I = -\frac{1}{2\pi}\oint \frac{e^{-ik(t-t')}}{(k-k_1)(k-k_2)}dk \quad \text{.......} \quad (9)$$

$$= -\frac{1}{2\pi}\int_{-K}^{+K} \frac{e^{-ik(t-t')}}{(k-k_1)(k-k_2)}dk - \frac{1}{2\pi}\int_{0}^{-\pi} \frac{e^{-iK(t-t')e^{i\phi}}}{(Ke^{i\phi}-k_1)(Ke^{i\phi}-k_2)} iKe^{i\phi}d\phi \quad \text{.......} \quad (10)$$

Where

$$k = Ke^{i\phi}, \; dk = iKe^{i\phi}d\phi$$

And ϕ lies between 0 and $-\pi$.

Now let K, the radius of the contour, become very large. Evaluating the integral by the residue theorem and inserting the values of k_1 and k_2 we get,

$$\mathrm{I} = -\frac{1}{2\pi}\lim_{K\to\infty} .\oint_c \frac{e^{-ik(t-t')}}{(k-k_1)(k-k_2)}dk \quad \text{.......} \quad (11)$$

$$= \frac{e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]}{\alpha} \quad \text{.......} \quad (12)$$

As $K \to \infty$, the first integral in Equation (10) on the right hand side will become just $G(t,t')$ of Equation (8). Thus we can write,

$$\frac{e^{-\frac{\mu(t-t')}{2}}\sin[\alpha(t-t')]}{\alpha} = G(t,t') + \lim_{K\to\infty}\left(-\frac{1}{2\pi}\right)\int_0^{-\pi}\frac{e^{-iK(t-t')e^{i\phi}}iKe^{i\phi}}{(Ke^{i\phi}-k_1)(Ke^{i\phi}-k_2)}d\phi \quad \text{......................... (13)}$$

Now the second term in Equation (13) vanishes as $K \to \infty$ by Jordan's Lema. Hence we get,

$$G(t,t') = \frac{e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]}{\alpha}(t > t') \quad \text{.. (14)}$$

But $G(t,t') = 0$ when $t < t'$

Thus in general we can write,

$$G(t,t') = \Theta(t-t')\frac{e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]}{\alpha} \quad \text{.. (15)}$$

Where $\Theta(t-t')$ is the Heaviside function? The general solution now becomes,

$$R_0(t) = PR_{01}(t) + QR_{02}(t) + \int_{t_0}^{t}\frac{e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]}{\alpha}f(t')dt' \quad \text{.................... (16)}$$

Where t_0 is the time at which the initial conditions may be applied, i.e., $f(t')$ may be taken to be zero at times prior to t_0.

The general solution to Equation (2) can be written in the form,

$$R(t) = C_1 + C_2e^{-\upsilon t} + \frac{B_0e^{-\beta t}}{\beta(\beta-\upsilon)} \quad \text{.. (17)}$$

Where C_1 and C_2 are constants.

Hence the value of $f(t')$ can be written as,

$$f(t') = \omega_0^2\left[C_1 + C_2e^{-\upsilon t'} + \frac{B_0e^{-\beta t'}}{\beta(\beta-\upsilon)}\right] + A_0e^{-\gamma t'} \quad \text{.................................... (18)}$$

Substituting the value of $f(t')$ from Equation (18) in Equation (16), we get,

$$R_0(t) = PR_{01}(t) + QR_{02}(t) + \frac{C_1\omega_0^2}{\alpha}\int_{t_0}^{t}e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]dt' + \frac{C_2\omega_0^2}{\alpha}\int_{t_0}^{t}e^{-\upsilon t'}e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]dt'$$

$$+\frac{B_0\omega_0^2}{\beta(\beta-\upsilon)\alpha}\int_{t_0}^{t}e^{-\beta t'}e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]dt' + \frac{A_0}{\alpha}\int_{t_0}^{t}e^{-\gamma t'}e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]dt' \quad \text{...........................(19)}$$

Or

$$R_0(t) = PR_{01}(t) + QR_{02}(t) + \frac{C_1\omega_0^2}{\alpha}I_1 + \frac{C_2\omega_0^2}{\alpha}I_2 + \frac{B_0\omega_0^2}{\beta(\beta-\upsilon)\alpha}I_3 + \frac{A_0}{\alpha}I_4 \quad \text{........................... (20)}$$

Where I_1, I_2, I_3 and I_4 are the four integrals of Equation (19). On evaluating these integrals and substituting them in Equation (19), we get,

$$R_0(t) = PR_{01}(t) + QR_{02}(t) + \frac{C_1\omega_0^2}{\alpha\left(\alpha^2+\frac{\mu^2}{4}\right)}\left[\alpha - e^{-\frac{\mu}{2}(t-t_0)}\left\{\frac{\mu}{2}\sin\alpha(t-t_0) + \alpha\cos\alpha(t-t_0)\right\}\right]$$

$$+\frac{C_2\omega_0^2e^{-\frac{\mu t}{2}}}{\alpha\left[\alpha^2+\left(\frac{\mu}{2}-\upsilon\right)^2\right]}\left[\alpha e^{\left(\frac{\mu}{2}-\upsilon\right)t} - e^{\left(\frac{\mu}{2}-\upsilon\right)t_0}\left\{\left(\frac{\mu}{2}-\upsilon\right)\sin\alpha(t-t_0) + \alpha\cos\alpha(t-t_0)\right\}\right]$$

$$+\frac{B_0\omega_0^2 e^{-\frac{\mu t}{2}}}{\alpha\beta(\beta-\upsilon)\left[\alpha^2+\left(\frac{\mu}{2}-\beta\right)^2\right]}\left[\alpha e^{\left(\frac{\mu}{2}-\beta\right)t}-e^{\left(\frac{\mu}{2}-\beta\right)t_0}\left\{\left(\frac{\mu}{2}-\beta\right)\sin\alpha(t-t_0)+\alpha\cos\alpha(t-t_0)\right\}\right]$$

$$+\frac{A_0 e^{-\frac{\mu t}{2}}}{\alpha\left[\alpha^2+\left(\frac{\mu}{2}-\gamma\right)^2\right]}\left[\alpha e^{\left(\frac{\mu}{2}-\gamma\right)t}-e^{\left(\frac{\mu}{2}-\gamma\right)t_0}\left\{\left(\frac{\mu}{2}-\gamma\right)\sin\alpha(t-t_0)+\alpha\cos\alpha(t-t_0)\right\}\right] \quad \text{.......................(21)}$$

The value of $R_0(t)$, apart from depending upon the variable t, depends on a number of other quantities, like $\omega_0,\mu,\upsilon,\gamma$ and β. In fact, the variables μ and υ are of the same nature, and γ and β are of the same nature. Note that at $t=t_0$, Equation (21) gives,

$$R_0(t)=PR_{01}(t)+QR_{02}(t) \quad \text{.......... (22)}$$

Which establishes the correctness of the solution given by Equation (21)?

Next we shall consider the solutions of Equations (1) and (2) by assuming that the forces $A(t)$ and $B(t)$ are oscillating, i.e.

$$A(t)=a_0 e^{-i\lambda t}$$
$$B(t)=b_0 e^{-i\psi t} \quad \text{.......... (23)}$$

Substituting for $A(t)$ and $B(t)$ in Equation (1) and (2), we get,

$$\ddot{R}_0(t)+\mu\dot{R}_0(t)+\omega_0^2 R_0(t)=a_0 e^{-i\lambda t}+\omega_0^2 R(t) \quad \text{.......... (24)}$$

$$\ddot{R}(t)+\upsilon\dot{R}(t)=b_0 e^{-i\psi t} \quad \text{.......... (25)}$$

The general solution for Equation (25) is,

$$R(t)=C_1+C_2 e^{-\upsilon t}-\frac{b_0 e^{-i\psi t}}{\psi(\psi-i\upsilon)} \quad \text{.......... (26)}$$

The Green's function for Equation (24) is similar to one given in Equation (15). The general solution of Equation (24) is

$$R_0(t)=MR_{01}(t)+NR_{02}(t)+\int\frac{e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]}{\alpha}F(t')dt' \quad \text{.......... (27)}$$

Where M and N are to be chosen to satisfy the boundary conditions, and

$$F(t')=a_0 e^{-i\lambda t'}+\omega_0^2 R(t')=a_0 e^{-i\lambda t'}+\omega_0^2\left[C_1+C_2 e^{-\upsilon t'}-\frac{b_0 e^{-i\psi t'}}{\psi(\psi-i\upsilon)}\right] \quad \text{.......... (28)}$$

Substituting the value of $F(t')$ from Equation (28) in Equation (27), we get,

$$R_0(t)=MR_{01}(t)+NR_{02}(t)+\frac{C_1\omega_0^2}{\alpha}\int_{t_0}^{t}e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]dt'$$

$$+\frac{C_2\omega_0^2}{\alpha}\int_{t_0}^{t}e^{-\upsilon t}e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]dt'-\frac{b_0\omega_0^2}{\psi(\psi-i\upsilon)\alpha}\int_{t_0}^{t}e^{-i\psi t'}e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]dt' \quad \text{........ (29)}$$

$$+\frac{a_0}{\alpha}\int_{t_0}^{t}e^{-i\lambda t}e^{-\frac{\mu}{2}(t-t')}\sin[\alpha(t-t')]dt'$$

On evaluating the integrals in Equation (29), we get

$$R_0(t) = MR_{01}(t) + NR_{02}(t) + \frac{C_1\omega_0^2}{\alpha\left(\alpha^2 + \frac{\mu^2}{4}\right)}\left[\alpha - e^{-\frac{\mu}{2}(t-t_0)}\left\{\frac{\mu}{2}\sin\alpha(t-t_0) + \alpha\cos\alpha(t-t_0)\right\}\right]$$

$$+ \frac{C_2\omega_0^2 e^{-\frac{\mu t}{2}}}{\alpha\left[\alpha^2 + \left(\frac{\mu}{2} - \upsilon\right)^2\right]}\left[\alpha e^{\left(\frac{\mu}{2}-\upsilon\right)t} - e^{\left(\frac{\mu}{2}-\upsilon\right)t_0}\left\{\left(\frac{\mu}{2} - \upsilon\right)\sin\alpha(t-t_0) + \alpha\cos\alpha(t-t_0)\right\}\right]$$

$$- \frac{b_0\omega_0^2 e^{-\frac{\mu t}{2}}}{\alpha\psi(\psi - i\upsilon)\left[\alpha^2 + \left(\frac{\mu}{2} - i\psi\right)^2\right]}\left[\alpha e^{\left(\frac{\mu}{2}-i\psi\right)t} - e^{\left(\frac{\mu}{2}-i\psi\right)t_0}\left\{\left(\frac{\mu}{2} - i\psi\right)\sin\alpha(t-t_0) + \alpha\cos\alpha(t-t_0)\right\}\right]$$

$$+ \frac{a_0 e^{-\frac{\mu t}{2}}}{\alpha\left[\alpha^2 + \left(\frac{\mu}{2} - i\lambda\right)^2\right]}\left[\alpha e^{\left(\frac{\mu}{2}-i\lambda\right)t} - e^{\left(\frac{\mu}{2}-i\lambda\right)t_0}\left\{\left(\frac{\mu}{2} - i\lambda\right)\sin\alpha(t-t_0) + \alpha\cos\alpha(t-t_0)\right\}\right] \text{.................}(30)$$

The value of $R_0(t)$ depends on the time variable t, and four other variables ω_0, μ, υ and λ along with ψ. the variables λ and ψ are of the same nature.

Again at $t = t_0$, Equation (30) gives that,

$$R_0(t) = MR_{01}(t) + NR_{02}(t) \text{ .... } (31)$$

Which establishes the correctness of the solution given in Equation (31)? The form of $R_0(t)$ in Equation (31) is the same as in Equation (22) except for the values of the co-efficient P and Q in Equation (22) and M and N in Equation (31). These coefficients can be chosen arbitrarily. The complete solutions giving the values of $R_0(t)$ are given by EQUATION (21) when the forces $\mathrm{A}(t)$ and $\mathrm{B}(t)$ are exponential, and then by Equation (30) when the forces are oscillatory. The values of $R_{01}(t)$ and $R_{02}(t)$ are given by Equation (7), and these values show that the exponential and oscillatory motions exist simultaneously. The phase difference between the motions represented by $R_{01}(t)$ and $R_{02}(t)$ is 90^0.

RESULTS AND DISCUSSION

To know how $R_0(t)$ varies with t we have to use Equations (22), (31) and (7). Apart from P, Q and M, N which may be treated as fixed, we need to know the values of the friction constant μ and the frequency ω_0. We can use the values used earlier (Cardi *et al.*, 1970) such that,

$$\mu = 1.06\times10^{-13}S^{-1} \text{ and } \omega_0^2 = 0.16\times10^{-26}S^{-2}$$

Equations (7) show that for $t = 0$, $R_{01}(t=0) = 0$ and $R_{02}(t=0) = 1$.This indicates that if $R_{01}(t=0)$ corresponds to the equilibrium position in the oscillation, and then $R_{02}(t=0)$ corresponds to the extreme position of the oscillation. But at $t = \infty$, $R_{01}(t=\infty) = 0$, and $R_{02}(t=\infty) = 0$, and this means that after a long time, the distinction between the position of equilibrium and the extreme position is lost, and the whole system will be in a state of equilibrium oscillating around the position R_{01}. The magnitudes of oscillation may be determined by P and Q. This means that even when the applied force is exponential, the oscillatory character predominates due to the form and nature of the Equations (1) and (2). Exactly similar results will be obtained from Equation (31). Therefore, it can be stated that the Green's function of solving the Equations (1) and (2) re-confirms that the itinerant oscillator model can be used for fluids.

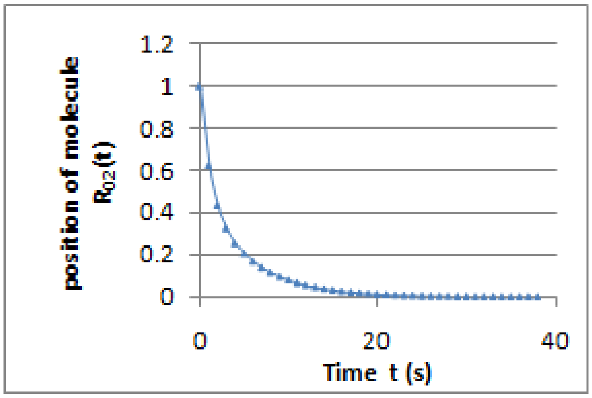

Figure 1: Variation of R_{02} with time t(s) for $\mu = 1.06\times10^{-13}s^{-1}$ **and** $\omega_0^2 = 0.16\times10^{-26}s^{-2}$

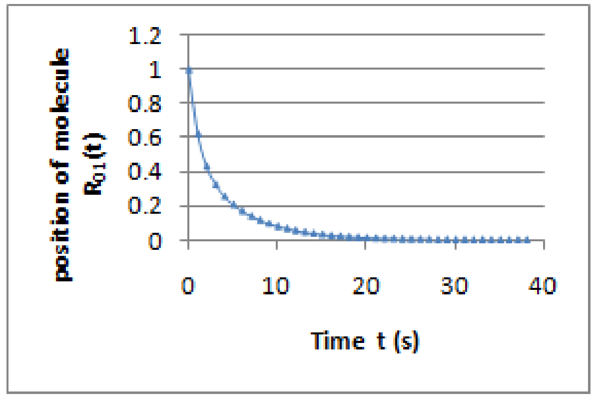

Figure 2: Variation of R_{01} with time t(s) for $\mu = 1.06\times10^{-13}s^{-1}$ **and** $\omega_0^2 = 0.16\times10^{-26}s^{-2}$

The graphs have been drawn for $R_{01}(t), R_{02}(t)$ and $R_0(t)$ for different values of μ and ω_0^2. All the graphs clearly indicate that under oscillatory damping forces, the displacement from the position of equilibrium dies as the time increases.

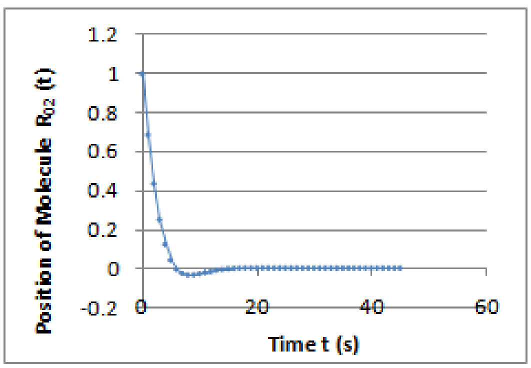

Figure 3: Variation of R_{02} with time t (s) for increased damping, $\mu = 0.68\times10^{-13}s^{-1}$; $\omega_0^2 = 0.188\times10^{-26}s^{-2}$

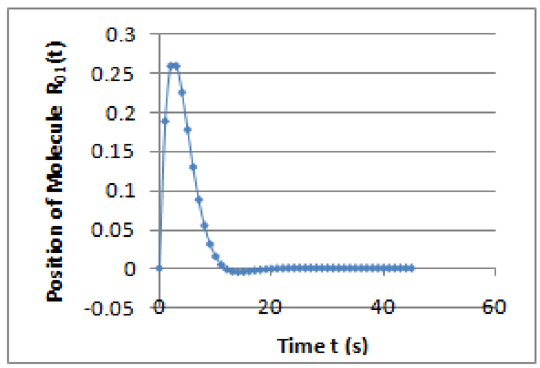

Figure 4: Variation of R_{01} with time t (s) for increased damping, $\mu = 0.68\times10^{-13}s^{-1}$; $\omega_0^2 = 0.188\times10^{-26}s^{-2}$

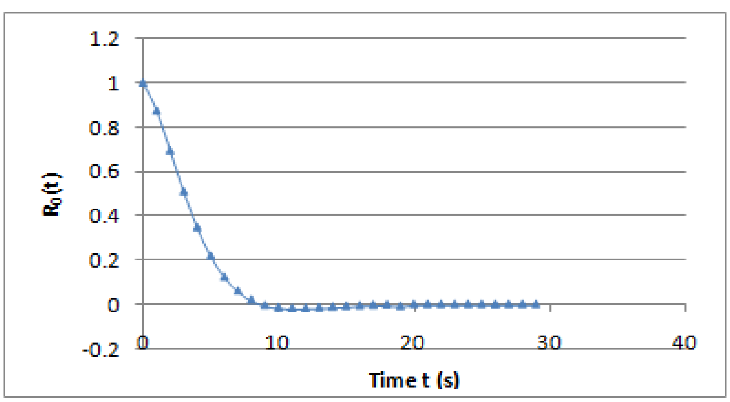

Figure 5: Variation of molecule displacement parameter R_0(t) with time t(s) for increased damping $\mu = 0.68\times10^{-13}s^{-1}$, $\omega_0^2 = 0.188\times10^{-26}s^{-2}$

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