Assignment 3 Applied Computational Science Derivation of Velocity-Velocity Correlation on Langevin Equation

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Problem 1. *We define:*

$$v(t) = v(0)\exp\big(-\frac{\gamma}{m}t\big) + \frac{1}{m}\int_0^t \exp\big(-\frac{\gamma}{m}(t-t')\big)\xi(t')dt' \tag{1}$$

Proof that:

$$< v(t_1)v(t_2) >= \frac{M}{m\gamma}\exp\big(-\frac{\gamma}{m}|t_1 - t_2|\big)$$

Proof.

$$\begin{aligned}
< v(t_1)v(t_2) > =& \big\langle v(0)\exp\big(-\frac{\gamma}{m}t_1\big) + \frac{1}{m}\int_0^{t_1}\exp\big(-\frac{\gamma}{m}(t_1 - t_1')\big)\xi(t_1')dt_1'\big\rangle \\
& \big\langle v(0)\exp\big(-\frac{\gamma}{m}t_2\big) + \frac{1}{m}\int_0^{t_2}\exp\big(-\frac{\gamma}{m}(t_2 - t_2')\big)\xi(t_2')dt_2'\big\rangle \\
=& \big\langle v(0)^2\big\rangle \exp\big(-\frac{\gamma}{m}(t_1+t_2)\big) + \frac{1}{m}\big\langle v(0)\int_0^{t_2}\exp\big(-\frac{\gamma}{m}(t_2 - t_2')\big)\xi(t_2')dt_2'\big\rangle \\
& + \frac{1}{m}\big\langle v(0)\int_0^{t_1}\exp\big(-\frac{\gamma}{m}(t_1 - t_1')\big)\xi(t_1')dt_1'\big\rangle \\
& + \frac{1}{m^2}\int_0^{t_1}dt_1'\int_0^{t_2}dt_2'\exp\big(-\frac{\gamma}{m}(t_1+t_2-t_1'-t_2')\big)\big\langle\xi(t_{1'})\xi(t_{2'})\big\rangle
\end{aligned}$$

We know that the mean value of a random force is equal to 0
, in that case, the terms
$\big\langle\xi(t_{1'})\big\rangle = 0$
and by using Ornstein - Uhlehnbeck Integration Method, the terms
$\big\langle\xi(t_{1'})\xi(t_{2'})\big\rangle = 2M\delta(t_1' - t_2')$

$$\begin{aligned}
< v(t_1)v(t_2) > =& \big\langle v(0)^2\big\rangle \exp\big(-\frac{\gamma}{m}(t_1+t_2)\big) \\
& + \frac{1}{m^2}\int_0^{t_1}dt_1'\int_0^{t_2}dt_2'\exp\big(-\frac{\gamma}{m}(t_1+t_2-t_1'-t_2')\big)2M\delta(t_1'-t_2')
\end{aligned}$$

We take $t_2' \approx t_1'$, hence the $\delta(t_1'-t_2')=0$ and the equation becomes:

$$
\begin{aligned}
< v(t_1)v(t_2) > =& \left\langle v(0)^2 \right\rangle \exp\big(-\frac{\gamma}{m}(t_1+t_2)\big) + \frac{1}{m^2}\int_0^{min(t_1,t_2)} dt_1' \exp\big(-\frac{\gamma}{m}(t_1+t_2-2t_1')\big)2M \\
=& \left\langle v(0)^2 \right\rangle \exp\big(-\frac{\gamma}{m}(t_1+t_2)\big) \\
& + \frac{2M}{m^2}\frac{m}{2\gamma}\left[\exp\big(-\frac{\gamma}{m}(t_1+t_2-2(min(t_1,t_2)))\big) - \exp\big(-\frac{\gamma}{m}(t_1+t_2)\big)\right]
\end{aligned}
$$

We use identity for simplify $(t_1+t_2-2(min(t_1,t_2))) = |t_1-t_2|$

And using equipartition theorem $\left\langle v(0)^2 \right\rangle = \dfrac{M}{m\gamma}$ the equation becomes:

$$
\begin{aligned}
< v(t_1)v(t_2) > =& \frac{M}{m\gamma}\exp\big(-\frac{\gamma}{m}(t_1+t_2)\big) + \frac{M}{m\gamma}\left[\exp\big(-\frac{\gamma}{m}|t_1-t_2|\big) - \exp\big(-\frac{\gamma}{m}(t_1+t_2)\big)\right] \\
=& \left[\frac{M}{m\gamma} - \frac{M}{m\gamma}\right]\exp\big(-\frac{\gamma}{m}(t_1+t_2)\big) + \frac{M}{m\gamma}\exp\big(-\frac{\gamma}{m}|t_1-t_2|\big) \\
< v(t_1)v(t_2) > =& \frac{M}{m\gamma}\exp\big(-\frac{\gamma}{m}|t_1-t_2|\big)
\end{aligned}
$$

$\square$