Computational Biophysics HW6

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1 Q1

We first find the coefficients as $\gamma\Delta t \to 0$. c_0 clearly approaches 1, and c_1 approaches 1 by L'Hopital's rule. Expanding c_2 in terms of $x \equiv \gamma\Delta t$ and using L'Hopital's rule twice we find:

$$c_2 = \left(\frac{1}{x}\left(1 - \frac{1}{x} + \frac{e^{-x}}{x}\right)\right)|_{x\to 0} \tag{1.1}$$

$$c_2 = \left(\frac{x + e^{-x} - 1}{x^2}\right)|_{x\to 0} \tag{1.2}$$

$$c_2 = \left(\frac{1 - e^{-x}}{2x}\right)|_{x\to 0} \tag{1.3}$$

$$c_2 = \left(\frac{e^{-x}}{2}\right)|_{x\to 0} \tag{1.4}$$

$$c_2 = \frac{1}{2} \tag{1.5}$$

σ_v^2 clearly approaches 0. Applying the same method above to σ_r^2 and ignoring the constants in front:

$$\sigma_r^2 = \frac{1}{x}\left(2 - \frac{1}{x}(3 - 4e^{-x} + e^{-2x})\right)|_{x\to 0} \tag{1.6}$$

$$\sigma_r^2 = \frac{2x - 3 + 4e^{-x} - e^{-2x}}{x^2}|_{x\to 0} \tag{1.7}$$

$$\sigma_r^2 = \frac{2 - 4e^{-x} + 2e^{-2x}}{2x}|_{x\to 0} \tag{1.8}$$

$$\sigma_r^2 = \frac{4e^{-x} - 4e^{-2x}}{2}|_{x\to 0} \tag{1.9}$$

$$\sigma_r^2 = 0 \tag{1.10}$$

A random variable drawn from a zero-mean Gaussian distribution with a variance of 0 is identically 0. Therefore our Langevin equations reduce to:

$$\mathbf{r}(t + \delta t) = \mathbf{r}(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2 \tag{1.11}$$

$$\mathbf{t} + \delta\mathbf{t} = v(t) + a(t)\delta t \tag{1.12}$$

These are just the inertial equations of motion, as we could see from the demonstration in class.

2 Q2

Taking the extreme limit as $\gamma\Delta t \to \infty$ it is clear that c_0, c_1 and c_2 all approach 0. σ_r^2 approaches 0, while σ_v^2 approaches $\frac{kT}{m}$. So the Langevin equations reduce to:

$$\mathbf{r}(t + \delta t) = \mathbf{r}(t) \tag{2.1}$$

$$\mathbf{t} + \delta\mathbf{t} = \Delta\mathbf{v}^G \tag{2.2}$$

So the particle can be modeled as having a random velocity at each point in time, with the variance of the speed being $\frac{kT}{m}$. The motion is therefore diffusive rather than inertial, and we expect the "random walk" trajectories we observed in class.

3 Q3

Using our results from Q1, we find the limit of equations 71 and 72:

$$\mathbf{r}(t + \delta t) = \mathbf{r}(t) + v(t)\delta t + \frac{1}{2}a(t)\delta t^2 \tag{3.1}$$

$$\mathbf{v}(t + \delta t) = v(t) + \frac{1}{2}a(t)\delta t + \frac{1}{2}a(t + \delta t)\delta t \tag{3.2}$$

$$\mathbf{v}(t + \delta t) = v(t) + \frac{1}{2}\delta t(a(t + \delta t) + a(t)) \tag{3.3}$$

These are the velocity Verlet equations.

4 Experiment

Gamma	Slope	D	T	T/gamma
5	1.1543	0.1924	1.0234	0.2047
6	0.9923	0.1654	1.0331	0.1722
7	0.8108	0.1351	1.0287	0.1470
8	0.7486	0.1248	1.0301	0.1288
9	0.6443	0.1074	1.0330	0.1148
10	0.5583	0.0931	1.0390	0.1309
12	0.4909	0.0818	1.0425	0.0869
15	0.3658	0.0610	1.0514	0.0701
20	0.2714	0.0452	1.0605	0.0530

The diffusion coeeficient may be estimated by $\frac{1}{6}\frac{dr^2}{dt}$, or through $D = \frac{kT}{m\gamma}$. The diffusion coefficient estimated from the mean squared displacement is plotted against T/γ below, and the slope of the line is 1 as expected.

Figure 1: Diffusion coefficient measured using alternate methods