Natural Sciences Tripos INSERT TITLE Supervision 1

Kirpal Grewal

2223-10-24

Q. 1.1

$$\boldsymbol{P} = \sum_{i=1}^{N} \boldsymbol{p}_i$$
$$\frac{d\boldsymbol{p}_i}{dt} = -\sum_{j\neq i}^{N} \frac{du(r_{ij})}{d_r} \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{r_{ij}}$$

ie the sum of all pairwise forces acting on the molecule

$$\frac{d\boldsymbol{P}}{dt} = \frac{d\boldsymbol{p}_i}{dt}$$

consider particles m and n and their force on each other

$$\frac{d\boldsymbol{p}_m}{dt} = -\frac{du(r_{nm})}{d_r} \frac{\boldsymbol{r}_n - \boldsymbol{r}_m}{r_{nm}}$$
$$\frac{d\boldsymbol{p}_m}{dt} = -\frac{du(r_{mn})}{d_r} \frac{\boldsymbol{r}_m - \boldsymbol{r}_n}{r_{mn}}$$

It can be seen that these have the same magnitude but oopposite direction and cancel each other out in the contribution to the overall potential: as we have assumed nothing about n and m this cancellation holds for all pairs of particles and the overall momentum of the system is time invariant

This follows from Noether's theorem as the system is invariant upon translation, the symmetry corresponding to conservation of the momentum of the system

Q. 1.2

For the leapfrog algorithm:

$$\begin{aligned}\boldsymbol{v}_i(t+\delta t/2) &= \boldsymbol{v}_i(t-\delta t/2) + \frac{\delta t}{m_i}\boldsymbol{f}_i(t)\\ \boldsymbol{r}_i(t+\delta t) &= \boldsymbol{r}_i(t) + \boldsymbol{v}_i(t+\delta t/2)\delta t\end{aligned}$$

$$\begin{aligned}\boldsymbol{r}_i(t+\delta t) &= \boldsymbol{r}_i(t) + \boldsymbol{v}_i(t+\delta t/2)\delta t\\ \boldsymbol{r}_i(t) &= \boldsymbol{r}_i(t-\delta t) + \boldsymbol{v}_i(t-\delta t/2)\delta t\\ \boldsymbol{r}_i(t+\delta t) - \boldsymbol{r}_i(t) &= \boldsymbol{r}_i(t) - \boldsymbol{r}_i(t-\delta t) + (\boldsymbol{v}_i(t+\delta t/2) - \boldsymbol{v}_i(t-\delta t/2))\delta t\end{aligned}$$

And substituting in the velocity change from the algorithm

$$\boldsymbol{r}_i(t+\delta t) - \boldsymbol{r}_i(t) = \boldsymbol{r}_i(t) - \boldsymbol{r}_i(t-\delta t) + \frac{\delta t^2}{m_i}\boldsymbol{f}_i(t)$$

The velocity Verlet

Q. 1.3

a

$$\begin{aligned}\langle A(t)\rangle &= \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \cos(\omega t)dt\\ &= \lim_{\tau\to\infty}\frac{1}{\omega\tau}\sin\omega\tau\\ &= 0\\ \langle A(t)^2\rangle &= \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \cos(\omega t)^2 dt\\ &= \lim_{\tau\to\infty}\frac{1}{4\omega\tau}(2\tau + \sin(2\tau\omega))\\ &= \frac{1}{2}\\ C_{AA}(t-t') &= \langle(\cos(\omega t))(\cos(\omega t'))\rangle\\ C_{AA}(\tau) &= \frac{1}{t}\int_0^\infty \cos(\omega t)(\cos(\omega(t-\tau)))dt\\ &= \frac{1}{t}\left[\frac{1}{2}t\cos(\omega\tau) - \frac{\sin(\omega(\tau-2t))}{4\omega}\right]\end{aligned}$$

Again the term in sin vanishes in the limit leaving

$$= \frac{1}{2}\cos(\omega\tau)$$

b

For any superposition of harmonic modes it is clear the time average will be 0

$$
\begin{aligned}
C_{AA}(\tau) &= \frac{1}{t}\int_0^\infty (a_1\cos(\omega_1 t) + a_2\cos(\omega_2 t))(a_1\cos(\omega_1(t-\tau)) + a_2\cos(\omega_2(t-\tau)))dt \\
&= \frac{a_1^2}{2}\cos(\omega_1\tau) + \frac{a_2^2}{2}\cos(\omega_2\tau) + \frac{a_1 a_2}{t}\int_0^\infty (\cos(\omega_1 t)\cos(\omega_2(t-\tau))) + (\cos(\omega_1(t-\tau))\cos(\omega_2 t))dt
\end{aligned}
$$

Using the orthogonality of sinusoidal functions of different frequencies, this integral is 0 in the limit

$$
= \frac{a_1^2}{2}\cos(\omega_1\tau) + \frac{a_2^2}{2}\cos(\omega_2\tau)
$$