

More on rotational motion of linear molecules

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In a previous article [1] I described the constraint algorithm for the rotational motion of rigid linear molecules. The orientation of the molecule is specified by \underline{e} , a unit vector along its axis. If the force centres are at positions $d_\alpha \underline{e}$ relative to the COM, the torque on the molecule is

$$\begin{aligned} \underline{T} &= \underline{e} \times \sum_{\alpha} d_{\alpha} \underline{f}_{\alpha} \\ &= \underline{e} \times \underline{G} \end{aligned}$$

By considering the motion of an 'equivalent diatomic' it is easily shown that the equation of motion (splitting into two first order equations) is

$$\dot{\underline{e}} = \underline{u} \tag{1a}$$

$$\dot{\underline{u}} = \underline{G}/I + \lambda \underline{e} \tag{1b}$$

where λ is an undetermined multiplier for the constraint force along the bond axis. My previous article solved this equation by using a simple leapfrog and then obtaining a quadratic equation for λ by using the constraint that the length of \underline{e} should remain unity. The purpose of this note is to give an alternative and simpler algorithm for integrating equation (1).

We first subtract out the component of \underline{G} parallel to \underline{e} i.e. replace \underline{G} by

$$\underline{G}_{\perp} = \underline{G} - (\underline{G} \cdot \underline{e}) \underline{e}$$

Writing a leapfrog for (1) then gives

$$\underline{u}^{n+\frac{1}{2}} = \underline{u}^{n-\frac{1}{2}} + \Delta t \underline{G}_{\perp}^n / I + \lambda \underline{e}^n \tag{2a}$$

$$\underline{e}^{n+1} = \underline{e}^n + \Delta t \underline{u}^{n+\frac{1}{2}} \tag{2b}$$

The reader may have noticed that since $G_{\underline{u}}$ has no component along \underline{e} the constraint force is required only to produce the centripetal acceleration, and in fact it can be shown that $\lambda = \underline{u}^2$. However we can obtain an algorithm without going through this step. The constraint on the bond length requires $\underline{u} \cdot \underline{e} = 0$; since we know \underline{e}^n we can use this if we have an estimate for \underline{u}^n . As explained in [2] where I discussed a similar equation for non-linear molecules the correct procedure is to use a first order expansion over $\frac{1}{2}\Delta t$ to obtain this estimate. Thus

$$\underline{u}^n = \underline{u}^{n-\frac{1}{2}} + \frac{1}{2}\Delta t \left[\underline{G}_{\underline{u}}^n / I + \lambda \underline{e}^n \right]$$

Then, using $\underline{G}_{\underline{u}}^n \cdot \underline{e}^n = 0$, $\underline{e}^n \cdot \underline{e}^n = 1$ and applying the constraint $\underline{u}^n \cdot \underline{e}^n = 0$ we find

$$0 = \underline{u}^{n-\frac{1}{2}} \cdot \underline{e}^n + \frac{1}{2}\Delta t \lambda$$

Substituting back for λ in (2a) gives

$$\underline{u}^{n+\frac{1}{2}} = \underline{u}^{n-\frac{1}{2}} - 2\underline{u}^{n-\frac{1}{2}} \cdot \underline{e}^n + \Delta t \underline{G}_{\underline{u}}^n / I \quad (3a)$$

Equations (3a) and (2b) then constitute a leapfrog type algorithm for the rotational motion, since we have expressed the centripetal acceleration in terms of the known quantities $\underline{u}^{n-\frac{1}{2}}$ and \underline{e}^n . In tests of this algorithm I have found that it gives identical results to the more complicated constraint algorithm of [1].

References

- 1 . D.Fincham, CCP5 Newsletter No.10, September 1983.
- 2 . D.Fincham, CCP5 Newsletter No.2, September 1981.