Solution to time-dependent problem

$$\frac{dW}{dt} = \hat{H}(t)W$$

$$W(t) = \mathcal{U}(t)W(0) \qquad \mathcal{U}(t) = T\left(e^{\int_0^t dt' H(t')}\right)$$

time-order exponential

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$$\mathcal{U}(t) = T\left(e^{\Delta t \sum_{k=0}^{n} H(k\Delta t)}\right) \qquad t = n\Delta t$$

$\Delta t \to 0$
$n\Delta t \to t$

$$= T\left(\prod_{k=0}^{n} e^{\Delta t H(k\Delta t)}\right)$$

$$= e^{\Delta t H(t)} e^{\Delta t H(t-\Delta t)} \cdots e^{\Delta t H(0)}$$

produce this result automatically

Suzuki's forward time-derivative operator

$$\hat{D} = \frac{\overleftarrow{\partial}}{\partial t}$$

$$F(t)\, e^{\Delta t \hat{D}} G(t) = F(t+\Delta t)\, G(t)$$

$$T\left(e^{\int_0^t H(s) ds} \right) = e^{t(\hat{H}(0)+\hat{D})} \qquad \boxed{n \Delta t = t}$$

$$= \left[e^{\Delta t (\hat{H}(0)+\hat{D})} \right]^n$$

$$\lim_{\substack{n \to \infty \\ \Delta t \to 0}} \quad = e^{\Delta t \hat{H}(0) + \Delta t \hat{D}}\, e^{\Delta t \hat{H}(0) + \Delta t \hat{D}} \cdots$$

$$= e^{\Delta t \hat{H}(0)}\, e^{\Delta t \hat{D}}\, e^{\Delta t \hat{H}(0)}\, e^{\Delta t \hat{D}} \cdots$$

$$= e^{\Delta t \hat{H}(\Delta t)}\, e^{\Delta t \hat{H}(0)}\, e^{\Delta t \hat{D}} \cdots$$

$$= e^{\Delta t \hat{H}(2\Delta t)}\, e^{\Delta t \hat{H}(\Delta t)}\, e^{\Delta t \hat{H}(0)}\, e^{\Delta t \hat{D}}$$

$$= e^{\Delta t \hat{H}(t)}\, e^{\Delta t \hat{H}(t-\Delta t)} \cdots$$

For the case $\hat{H}(t) = \hat{T} + \hat{V}(t)$

$$T\left(e^{\int_0^{\Delta t}\hat{H}(s)ds}\right) = e^{\Delta t(\hat{H}(0)+\hat{D})}$$
$$= e^{\Delta t(\hat{T}+\hat{D}+\hat{V}(0))}$$

For Cromer's algorithm

Since $\hat{T}$ is time-independent $[\hat{T},\hat{D}]=0$

$$e^{\Delta t(\hat{T}+\hat{D}+\hat{V}(0))} \approx e^{\Delta t\hat{T}+\Delta t\hat{D}} e^{\Delta t\hat{V}(0)}$$

$$e^{\Delta t\hat{D}} e^{\Delta t\hat{T}} \nearrow \begin{pmatrix} q \\ v \end{pmatrix}$$

$$= \underline{e^{\Delta t\hat{D}} e^{\Delta t\hat{T}}} e^{\Delta t\hat{V}(0)}$$

$v \equiv \frac{p}{m}$

$$= e^{\Delta t\hat{D}} e^{\Delta t\hat{T}} \begin{pmatrix} q \\ v+\Delta t\, a(q,0) \end{pmatrix}$$

$$e^{\Delta t\hat{D}} \begin{pmatrix} q+v\Delta t \\ v+\Delta t\, a(q+v\Delta t,0) \end{pmatrix}$$

$t=0$

$$t = t+\Delta t$$

Since $\hat{D}$ is combine with $\hat{T}$ with the same $a_i\Delta t$ step, every $\hat{T}$ needs a time update $t + a_i\Delta t$.

effect is

1b

$$q_1 = q + v\Delta t$$
$$v_1 = v + \Delta t\, a(q_1,t)$$

Compare to

$$q_1 = q+v\Delta t$$
$$t = t+\Delta t$$
$$v_1 = v+\Delta t\, a(q_1,t)$$

equivalent! to 1a given previously

$$\left.\begin{array}{l} q_1 = q+v\Delta t \\ v_1 = v+\Delta t\, a(q,t) \end{array}\right\} 1a$$
$$q_2 = q_1 + v_1\Delta t$$
$$v_2 = v_1 + \Delta t\, a(q_2, t+\Delta t)$$
$$\vdots$$

Also second-order algorithm given previously

Also higher-order symplectic algorithms

$$T_4(\Delta t) = T_2\left(\frac{\Delta t}{2-s}\right) T_2\left(-\frac{\Delta t\, s}{2-s}\right) T_2\left(\frac{\Delta t}{2-s}\right)$$

det M = 1

$$s = 2^{1/3}$$

holds true for time-dependent case.

Higher-order Runge-Kutta algorithm

$$T_2 = e^{\Delta t \hat{H} + \Delta t^3 \hat{E}_3 + \cdots}$$

$$RK_2 = \frac{1}{2}\left(T_{1a}(\Delta t) + T_{1b}(\Delta t)\right)$$

det M ≠ 1

$$\boxed{RK_4 = \frac{1}{3}\left(4 T_2\left(\frac{\Delta t}{2}\right) T\left(\frac{\Delta t}{2}\right) - T_2(\Delta t)\right)}$$

$$= \frac{1}{3}\left(4\left(1 + \frac{\Delta t}{2}\hat{H} + \left(\frac{\Delta t}{2}\right)^3 \hat{E}_3\right)^2 - \left(1 + \Delta t \hat{H} + \Delta t^3 \hat{E}_3 \cdots\right)\right)$$

$$= \frac{1}{3}\left(4\left(1 + \Delta t \hat{H} + + \frac{\Delta t^3}{4}\hat{E}_3 + \cdots\right) - (\quad)\right)$$

$$= \frac{1}{3}\left(3 + 3\Delta t \hat{H} + \cdots\right)$$

$$= 1 + \Delta t \hat{H} + \cdots = e^{\Delta t \hat{H} + \Delta t^5 \hat{H} + \cdots}$$

exactly the same as RK_4 as given before! $\Delta t \to 0$!

Higher-order Runge-Kutta

$$RK_6(\Delta t) = \frac{1}{24} T_2(\Delta t) - \frac{16}{15} T_2^2(\Delta t/2) + \frac{81}{90} T_2^3(\Delta t/3)$$

etc., etc.,

can solve any time-ind or time-depend problem to any order in Δt.

symplect algorithm $\propto 3^n$

Runge-Kutta $\propto n^2$