Nosé–Hoover Chains

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Contents

1 Introduction

Well, and here begins my lovely article. [**?**]

2 Numerical integrating the Nosé–Hoover chain equations

the thermostat forces in eqn.(4.11.6) vary rapidly
employing a higher-order factorization

2.1 Suzuki–Yoshida scheme

$$\sum_{\alpha=1}^{n_{\text{sy}}} w_\alpha = 1$$

1. You can nest the list environments to your taste:
   - fourth-order scheme
   $$w_1 = w_3 = \frac{1}{2-2^{1/3}} w_2 = \quad 1 - w_1 - w_3.$$
   - sixth-order scheme
   $$\begin{aligned} w_1 =& w_7 = 0.784513610477560 \\ w_2 =& w_6 = 0.235573213359357 \\ w_3 =& w_5 = -1.1767998417887 \\ w_4 =& 1 - w_1 - w_2 - w_3 - w_5 - w_6 - w_6 - w_7 - w_7. \end{aligned}$$
2. Therefore remember:

Using the Suzuki–Yoshida scheme allows the propagator in eqn. (4.11.8) to be written as

$$\mathrm{e}^{iL\Delta t} \approx \prod_{\beta=1}^{n_{\text{sy}}} \left[S\left(w_\beta \Delta t/2n\right)\right]^n \mathrm{e}^{iL_2\Delta t/2} \mathrm{e}^{iL_1\Delta t} \mathrm{e}^{iL_2\Delta t/2} \prod_{\alpha=1}^{n_{\text{sy}}} \left[S\left(w_\alpha \Delta t/2n\right)\right]^n$$

One scheme in particular, due to Suzuki(1991a, 1991b) and Yoshida(1990), has proved particularly useful for the Nosé–Hoover chain system.

… and here it ends.

3 Numerical evolution

$$
\begin{aligned}
\exp\left(cx\frac{\partial}{\partial x}\right) f(x) &= \left[\sum_{m=0}^{\infty}\frac{c^m}{m!}\left(x\frac{\partial}{\partial x}\right)^m\right]\left[\sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}x^n\right] \\
&= \sum_{n=0}^{\infty}\frac{f^{(n)}(0)}{n!}\sum_{m=0}^{\infty}\frac{n!c^m x^{n-m}}{m!(n-m)!} \\
&= f(x\mathrm{e}^c)
\end{aligned}
$$

Here, we show the approximated numerical evolution in detail. The classical propagator in a single step is

$$
\mathrm{e}^{iL\Delta t} \approx \prod_{\beta=1}^{n_{\mathrm{sy}}}\left[S\left(w_\beta \Delta t/2n\right)\right]^n \mathrm{e}^{iL_2\Delta t/2}\mathrm{e}^{iL_1\Delta t}\mathrm{e}^{iL_2\Delta t/2}\prod_{\alpha=1}^{n_{\mathrm{sy}}}\left[S\left(w_\alpha \Delta t/2n\right)\right]^n .
$$

$$
\exp\left(\frac{w_\alpha \Delta t}{4n}F_{\eta,M}\frac{\partial}{\partial p_{\eta,M}}\right)\begin{pmatrix}\vdots \\ p_{\eta,M} \\ \vdots\end{pmatrix} = \begin{pmatrix}\vdots \\ p_{\eta,M} + \frac{w_\alpha \Delta t}{4n}F_{\eta,M} \\ \vdots\end{pmatrix}
$$

$$
\begin{aligned}
&\exp\left(-\frac{\delta_\alpha}{8}\frac{p_{\eta,j+1}}{m_{\eta,j+1}}p_{\eta,j}\frac{\partial}{\partial p_{\eta,j}}\right)\exp\left(\frac{\delta_\alpha}{4}F_{\eta,j}\frac{\partial}{\partial p_{\eta,j}}\right)\exp\left(-\frac{\delta_\alpha}{8}\frac{p_{\eta,j+1}}{m_{\eta,j+1}}p_{\eta,j}\frac{\partial}{\partial p_{\eta,j}}\right)\begin{pmatrix}\vdots \\ p_{\eta,j} \\ \vdots\end{pmatrix} \\
=&\exp\left(-\frac{\delta_\alpha}{8}\frac{p_{\eta,j+1}}{m_{\eta,j+1}}p_{\eta,j}\frac{\partial}{\partial p_{\eta,j}}\right)\exp\left(\frac{\delta_\alpha}{4}F_{\eta,j}\frac{\partial}{\partial p_{\eta,j}}\right)\begin{pmatrix}\vdots \\ p_{\eta,j}\exp\left(-\frac{\delta_\alpha}{8}\frac{p_{\eta,j+1}}{m_{\eta,j+1}}\right) \\ \vdots\end{pmatrix} \\
=&\exp\left(-\frac{\delta_\alpha}{8}\frac{p_{\eta,j+1}}{m_{\eta,j+1}}p_{\eta,j}\frac{\partial}{\partial p_{\eta,j}}\right)\begin{pmatrix}\vdots \\ p_{\eta,j}\exp\left(-\frac{\delta_\alpha}{8}\frac{p_{\eta,j+1}}{m_{\eta,j+1}}\right)+\frac{\delta_\alpha}{4}F_{\eta,j} \\ \vdots\end{pmatrix} \\
=&\begin{pmatrix}\vdots \\ p_{\eta,j}\exp\left(-\frac{\delta_\alpha}{4}\frac{p_{\eta,j+1}}{m_{\eta,j+1}}\right)+\frac{\delta_\alpha}{4}F_{\eta,j} \\ \vdots\end{pmatrix}
\end{aligned}
$$

$$
\exp\left(-\frac{\delta_\alpha}{2}\frac{p_{\eta,j}}{m_{\eta,j}}\frac{\partial}{\partial r_{\eta,j}}\right)\begin{pmatrix}\vdots \\ r_{\eta,j} \\ \vdots\end{pmatrix} = \begin{pmatrix}\vdots \\ r_{\eta,j} - \frac{\delta_\alpha}{2}\frac{p_{\eta,j}}{m_{\eta,j}} \\ \vdots\end{pmatrix}
$$

$$
\exp\left(-\frac{\delta_\alpha}{2}\frac{p_{\eta,1}}{m_{\eta,1}}p_i\cdot\frac{\partial}{\partial p_i}\right)\begin{pmatrix}\vdots \\ p_i \\ \vdots\end{pmatrix} = \begin{pmatrix}\vdots \\ p_i\exp\left(-\frac{\delta_\alpha}{2}\frac{p_{\eta,1}}{m_{\eta,1}}\right) \\ \vdots\end{pmatrix}
$$

References