### A. Algorithm for BKNHC chain dynamics

Splitting the BKNHC chain Hamiltonian as

$$H_1^{\text{BKNHC}} = V(q) \tag{47a}$$

$$H_2^{\text{BKNHC}} = \frac{p^2}{2m} \tag{47b}$$

$$H_3^{\text{BKNHC}} = k_B T\zeta \tag{47c}$$

$$H_4^{\text{BKNHC}} = k_B T\xi \tag{47d}$$

$$H_5^{\text{BKNHC}} = \frac{K_1(p_\zeta)}{m_\zeta} \tag{47e}$$

$$H_6^{\text{BKNHC}} = \frac{K_2(p_\xi)}{m_\xi} \tag{47f}$$

$$H_7^{\text{BKNHC}} = \frac{p_\eta^2}{2m_\eta} \tag{47g}$$

$$H_8^{\text{BKNHC}} = k_B T\eta \tag{47h}$$

$$H_9^{\text{BKNHC}} = \frac{p_\chi^2}{2m_\chi} \tag{47i}$$

$$H_{10}^{\text{BKNHC}} = k_B T\chi \;, \tag{47j}$$

we obtain the corresponding measure-preserving splitting of the Liouville operator

$$L_\alpha = \mathcal{B}_{ij}^{\text{BKNHC}} \frac{\partial H_\alpha^{\text{BKNHC}}}{\partial x_j} \frac{\partial}{\partial x_i}. \tag{48}$$

At this stage we go directly to Eqs (20). The antisymmetric Nosé-Hoover-Bulgac-Kusnezov tensor becomes

$$\tilde{\boldsymbol{\mathcal{B}}}^{\text{BKNHC}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & -q & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 & 0 & -p & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & p & 0 & 0 & -p_\zeta & 0 \\ q & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -p_\xi \\ 0 & 0 & 0 & -1 & 0 & 0 & p_\zeta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & p_\xi & 0 & 0 \end{bmatrix} , \tag{49}$$