

Appendix B

Implementation of the dissipative CCDM equations

In this Appendix, it is shown how Eqn.(5.34) can be recast in a form which leads to a scaling of the numerical effort of $O(K^3 \times N^2)$. Eqn.(5.34) is

$$\begin{aligned}
\dot{\rho}_{D,kl}^{rs} &= \sqrt{f(Z_r) \cdot f(Z_s)} \sum_{\alpha\beta=0}^{K-1} \sum_{ij=0}^{K-1} \Gamma_{\alpha_c\beta_c} S_{k\alpha_r} S_{\beta_r i} \rho_{ij}^{rs} S_{j\beta_s} S_{\alpha_s l} \\
&\quad - \frac{1}{2} f(Z_r) \sum_{\alpha\beta=0}^{K-1} \sum_{ij=0}^{K-1} \Gamma_{\alpha_c\beta_c} S_{k\beta_r} S_{\alpha_r i} S_{i\alpha_r} S_{\beta_r j} \rho_{jl}^{rs} \\
&\quad - \frac{1}{2} f(Z_s) \sum_{\alpha\beta=0}^{K-1} \sum_{ij=0}^{K-1} \Gamma_{\alpha_c\beta_c} \rho_{ki}^{rs} S_{i\beta_s} S_{\alpha_s j} S_{j\alpha_s} S_{\beta_s l} \\
&:= \dot{\rho}_{D,kl}^{rs}(1) + \dot{\rho}_{D,kl}^{rs}(2a) + \dot{\rho}_{D,kl}^{rs}(2b) \quad ,
\end{aligned} \tag{B.1}$$

Let us consider the term $\dot{\rho}_{D,kl}^{rs}(1)$ first. Introducing the matrix

$$R_{\alpha\beta}^{\mu\nu,r} := \langle \mu_r | \alpha_r \rangle \langle \beta_r | \nu_r \rangle \tag{B.2}$$

and using $|\alpha_r\rangle = \sum_{\beta} |\beta_r\rangle \langle \beta_r | \alpha_r \rangle$, we get

$$\begin{aligned}
\dot{\rho}_{D,kl}^{rs}(1) &= \sqrt{f(Z_r) f(Z_s)} \sum_{\alpha\beta=0}^{K-1} \Gamma_{\alpha_c\beta_c} \sum_{ij=0}^{K-1} \sum_{\mu\nu\sigma\lambda} S_{k\mu_r} R_{\alpha\beta}^{\mu\nu,r} S_{\nu_r i} \rho_{ij}^{rs} S_{j\sigma_s} R_{\beta\alpha}^{\sigma\lambda,s} S_{\lambda_s l} \\
&= \sqrt{f(Z_r) f(Z_s)} \sum_{\mu\lambda} S_{k\mu_r} \left[\sum_{\alpha\beta=0}^{K-1} \sum_{\nu\sigma} \Gamma_{\alpha_c\beta_c} R_{\alpha\beta}^{\mu\nu,r} \left\{ \sum_{ij=0}^{K-1} S_{\nu_r i} \rho_{ij}^{rs} S_{j\sigma_s} \right\} R_{\beta\alpha}^{\sigma\lambda,s} \right] S_{\lambda_s l} \\
&=: \sqrt{f(Z_r) f(Z_s)} \sum_{\mu\lambda} S_{k\mu_r} \left[\sum_{\alpha\beta=0}^{K-1} \sum_{\nu\sigma} \Gamma_{\alpha_c\beta_c} R_{\alpha\beta}^{\mu\nu,r} U_{\nu\sigma}^{rs} R_{\beta\alpha}^{\sigma\lambda,s} \right] S_{\lambda_s l} \quad ,
\end{aligned} \tag{B.3}$$

where

$$U_{\nu\sigma}^{rs} := \sum_{ij=0}^{K-1} S_{\nu r i} \rho_{ij}^{rs} S_{j\sigma s} \quad . \quad (\text{B.4})$$

Considering the orthonormality relations $R_{\alpha\beta}^{\mu\nu,r} = \delta_{\mu\alpha}\delta_{\beta\nu}$, we have

$$\begin{aligned} \dot{\rho}_{D,kl}^{rs}(1) &= \sqrt{f(Z_r)f(Z_s)} \sum_{\alpha\beta=0}^{K-1} S_{k\alpha r} \Gamma_{\alpha_c\beta_c} U_{\beta\beta}^{rs} S_{\alpha_s l} \\ &= \sqrt{f(Z_r)f(Z_s)} \sum_{\beta=0}^{K-1} U_{\beta\beta}^{rs} \sum_{\alpha=0}^{K-1} S_{k\alpha r} S_{\alpha_s l} \Gamma_{\alpha_c\beta_c} \\ &=: \sum_{\beta=0}^{K-1} A_{\beta}^{rs} \cdot B_{\beta,kl}^{rs} \\ &= \mathbf{A}^{rs\dagger} \cdot \mathbf{B}_{kl}^{rs} \quad , \end{aligned} \quad (\text{B.5})$$

where

$$A_{\beta}^{rs} := U_{\beta\beta}^{rs} \quad (\text{B.6})$$

$$B_{\beta,kl}^{rs} := \sqrt{f(Z_r)f(Z_s)} \sum_{\alpha=0}^{K-1} S_{k\alpha r} S_{\alpha_s l} \Gamma_{\alpha_c\beta_c} \quad . \quad (\text{B.7})$$

Note that the (row) vector $\mathbf{A}^{rs\dagger}$, defined by Eqn. (B.6) and used in Eqn. (B.5), does not depend on (k,l); it must therefore be evaluated only once and can then be used for every combination (k,l). However, since it contains the actual density matrix, this has to be done for every timestep. For each element A_{β}^{rs} , $\propto K^2$ multiplications are required. Since each vector \mathbf{A}^{rs} contains K elements, and since there are $N \times N$ vectors of this type, the scaling arising from evaluating these vectors is $\propto K^3 N^2$. The (column) vector \mathbf{B}_{kl}^{rs} depends on the state indices, and has to be computed for each combination (k,l), but only once at the beginning of the propagation cycle. (The computation of each individual element \mathbf{B}_{kl}^{rs} , requires K operations.) Hence, the algorithm to evaluate $\dot{\rho}_D(1)$ requires $O(K^3 \cdot N^2)$ operations.

The second term $\dot{\rho}_{D,kl}^{rs}(2)$ occurring in Eqn.(B.1) can be simplified along similar lines. We consider only the term $\dot{\rho}_{D,kl}^{rs}(2a)$, because the term $\dot{\rho}_{D,kl}^{rs}(2b)$ can be

manipulated in analogous fashion. We have

$$\begin{aligned}
\dot{\rho}_{D,kl}^{rs}(2a) &= -\frac{1}{2} \sum_{\alpha\beta=0}^{K-1} \Gamma_{\alpha_c\beta_c} \cdot f(Z_r) \sum_{ij=0}^{K-1} S_{k\beta_r} S_{\alpha_r i} S_{i\alpha_r} S_{\beta_r j} \rho_{jl}^{rs} \\
&= -\frac{1}{2} \sum_{j=0}^{K-1} D_{kj}^{rs} \rho_{jl}^{rs} \\
&= -\frac{1}{2} (\mathbf{D}^{rs} \boldsymbol{\rho}^{rs})_{kl} \quad .
\end{aligned} \tag{B.8}$$

The matrix \mathbf{D}^{rs} with elements

$$D_{kj}^{rs} := \sum_{\alpha\beta=0}^{K-1} \sum_{i=0}^{K-1} \Gamma_{\alpha_c\beta_c} \cdot f(Z_r) S_{k\beta_r} S_{\alpha_r i} S_{i\alpha_r} S_{\beta_r j} \tag{B.9}$$

has to be computed only once at the beginning of the propagation cycle. (For this purpose, $\propto K^4 N^2$ operations are required.) Following this, in each timestep for each matrix element $\dot{\rho}_{D,kl}^{rs}(2a)$, only K additional multiplications are required.

Hence, the overall scaling for the “dissipative operation” $\mathcal{L}_D(\hat{\rho})$ in the dissipative Liouville-von Neumann equation (2.9) for this CCDM formulation is $O(K^3 \cdot N^2)$.