

CDVR Algorithm

The CDVR algorithm (Manthe JCP 1996 **105**: 6989) is a time dependent DVR with a correction to treat separable components of the Hamiltonian exactly.

We have three bases:

The SPF basis $|\varphi_{j_\kappa}^{(\kappa)}\rangle$

The DVR basis on the points x , $|X_{x_\kappa}^{(\kappa)}\rangle$

The TDDVR basis on the points q , $|Q_{q_\kappa}^{(\kappa)}\rangle$

where the latter are the eigenvalues $q^{(\kappa)}$ and eigenvectors $U_{qj}^{(\kappa)} = \langle Q_q^{(\kappa)} | \varphi_j^{(\kappa)} \rangle$ of the position operator in the spf basis $\langle \varphi_j^{(\kappa)} | x | \varphi_m^{(\kappa)} \rangle$. The matrix $D_{qj}^{(\kappa)} = \langle X_q^{(\kappa)} | \varphi_j^{(\kappa)} \rangle$ is the definition of the SPF basis in the DVR basis.

To evaluate a matrix element in the TDDVR basis:

$$\langle Q_{j_1}^{(1)} \cdots Q_{j_f}^{(f)} | V(x_1, \dots, x_f) | Q_{m_1}^{(1)} \cdots Q_{m_f}^{(f)} \rangle = V(q_{j_1}^{(1)} \cdots q_{j_f}^{(f)}) \delta_{j_1 m_1} \cdots \delta_{j_f m_f} +$$

$$\sum_{\kappa=1}^f \langle Q_{m_\kappa}^{(\kappa)} | \Delta V(q_{j_1}^{(1)} \cdots q_{j_{\kappa-1}}^{(\kappa-1)}, x_\kappa, q_{j_{\kappa+1}}^{(\kappa+1)} \cdots q_{j_f}^{(f)}) | Q_{m_\kappa}^{(\kappa)} \rangle \delta_{j_1 m_1} \cdots \delta_{j_{\kappa-1} m_{\kappa-1}} \delta_{j_{\kappa+1} m_{\kappa+1}} \cdots \delta_{j_f m_f}$$

where the first term on the RHS is the approximation that the potential is diagonal

on the TDDVR points, and the second term is the CDVR correction: $\langle Q_{m_\kappa}^{(\kappa)} | \Delta V(q_{j_1}^{(1)} \cdots q_{j_{\kappa-1}}^{(\kappa-1)}, x_\kappa, q_{j_{\kappa+1}}^{(\kappa+1)} \cdots q_{j_f}^{(f)}) \rangle$

$$\langle Q_{m_\kappa}^{(\kappa)} | V(q_{j_1}^{(1)} \cdots q_{j_{\kappa-1}}^{(\kappa-1)}, x_\kappa, q_{j_{\kappa+1}}^{(\kappa+1)} \cdots q_{j_f}^{(f)}) | Q_{m_\kappa}^{(\kappa)} \rangle - V(q_{j_1}^{(1)} \cdots q_{j_f}^{(f)}) \delta_{j_\kappa m_\kappa}$$

MCTDH Code

In **getcdvr**, the $q^{(\kappa)}$ and $U_{qj}^{(\kappa)}$ are calculated and stored for each mode.

In **matrizen4** the mean fields and time derivative of the A-coefficients is calculated, using the CDVR method.

1. Transform coefficients from spf to TDDVR basis:

$$B_{q_1 \cdots q_f} = \sum_j U_{qj}^{(1)} \cdots U_{qj}^{(f)} A_{j_1 \cdots j_f}$$

2. Calculate mean fields and CDVR correction.

do $\kappa = 1, f$

- (i) transform mode κ from TDDVR to DVR basis

$$B'_{q_1 \cdots, x_\kappa, \cdots, q_f} = D_{xj}^{(\kappa)} U_{qj}^{(\kappa)\dagger} B_{q_1 \cdots q_\kappa \cdots q_f}$$

- (ii) operate on B

$$B_{q_1 \cdots, x_\kappa, \cdots, q_f}^V = V(q_1 \cdots, x_\kappa, \cdots, q_f) B'_{q_1 \cdots, x_\kappa, \cdots, q_f}$$

- (iii) form meanfield matrix

$$H(x, q) = \sum B_{q_1 \cdots, q_\kappa, \cdots, q_f}^* B_{q_1 \cdots, x_\kappa, \cdots, q_f}^V$$

$$H(x, j) = U_{qj}^{(\kappa)\dagger} H(x, q)$$

- (iv) Calculate CDVR correction

$$C_{q_1 \cdots, q_\kappa, \cdots, q_f} = U_{q,j}^{(\kappa)} D_{x,j}^{(\kappa)} B_{q_1 \cdots, x_\kappa, \cdots, q_f}^V$$

enddo

3. calculate

$$V_{q_1 \cdots, q_\kappa, \cdots, q_f} = V(q_{j_1}^{(1)} \cdots q_{j_f}^{(f)})$$

4. calculate

$$i\dot{A}'_{q_1 \cdots, q_\kappa, \cdots, q_f} = C_{q_1 \cdots, q_\kappa, \cdots, q_f} - (f-1)V_{q_1 \cdots, q_\kappa, \cdots, q_f}$$

5. transform A from TDDVR to SPF basis

$$i\dot{A}_{j_1 \cdots j_f} = \sum_j U_{qj}^{(1)\dagger} \cdots U_{qj}^{(f)\dagger} A'_{q_1 \cdots q_f}$$